UNIVERSIDADE FEDERAL DO RIO GRANDE DO SUL

ESCOLA DE ENGENHARIA

DEPARTAMENTO DE ENGENHARIA QUÍMICA

PROGRAMA DE PÓS-GRADUAÇÃO EM ENGENHARIA QUÍMICA

Síntese Simultânea de Redes de Trocadores de Calor com considerações Operacionais: Flexibilidade e Controlabilidade

TESE DE DOUTORADO

Marcelo Escobar Aragão

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Tese de Doutorado apresentada como requisito parcial para obtenção do título de Doutor em Engenharia.

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A Comissão Examinadora, abaixo assinada, aprova a Tese *Síntese Simultânea de Redes de Trocadores de Calor com considerações Operacionais: Flexibilidade e Controlabilidade*, elaborada por Marcelo Escobar Aragão, como requisito parcial para obtenção do título de Doutor em Engenharia.

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“Gosto dos venenos mais lentos, das bebidas mais amargas, das drogas mais poderosas, das idéias mais insanas, dos pensamentos mais complexos, dos sentimentos mais fortes… tenho um apetite voraz e os delírios mais loucos.
Você pode até me empurrar de um penhasco que eu vou dizer:
- E daí? Eu adoro voar!
Não me mostrem o que esperam de mim, por que vou seguir meu coração. Não me façam ser quem não sou. Não me convidem a ser igual, por que sinceramente sou diferente. Não sei amar pela metade. Não sei viver de mentira. Não sei voar de pés no chão. Sou sempre eu mesmo, mas com certeza não serei o mesmo pra sempre.”

Clarice Lispector

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Resumo

Neste trabalho foi desenvolvido um procedimento computacional para síntese de redes de trocadores de calor que sejam flexíveis (capazes de operar sujeito a incerteza) e controláveis. A síntese foi baseada em uma superestrutura proposta na literatura que tem como objetivo minimizar simultaneamente o custo operacional e de investimento do projeto. Considerações gerais baseadas nessa formulação foram discutidas neste trabalho. Assumiu-se incerteza nas temperaturas de entrada e vazões de cada corrente. Inicialmente foi implementado um procedimento para geração de projetos flexíveis baseado numa estratégia em dois estágios. O primeiro estágio precede a operação (fase de projeto) onde as variáveis de projeto são escolhidas, i.e. a existência e a dimensão dos equipamentos. Num segundo estágio (fase de operação) as variáveis de controle, i.e. os graus de liberdade adicionais, são ajustados de acordo com a realização dos parâmetros incertos. O estágio de projeto é realizado através de um problema de otimização multiperíodo, onde cada período corresponde a um cenário operacional, resultando em um problema do tipo MINLP. Com o objetivo de explorar a estrutura bloco-diagonal de problemas dessa natureza, uma técnica de decomposição baseada no conceito de relaxação Lagrangeana foi desenvolvida como uma alternativa para resolução de problemas de larga escala. A etapa de operação consiste numa análise de Flexibilidade tendo como objetivo checar se o projeto obtido no estágio anterior é capaz de operar na região de incerteza especificada. Esta análise é realizada através da avaliação do Índice de Flexibilidade, através da estratégia do conjunto ativo resultando em um problema MI(N)LP. Caso o projeto seja suficientemente flexível, passa-se para a etapa seguinte, caso contrário, o ponto crítico que define a solução desse problema é adicionado ao conjunto inicial de cenários operacionais e o problema multiperíodo é resolvido novamente. Este procedimento é resolvido iterativamente até que se tenha um projeto flexível. Neste caso, um problema MILP é resolvido com o intuito de selecionar a estrutura de controle, baseado na minimização de métricas de controlabilidade, que garantem manter as temperaturas de saída em suas respectivas referências usando controladores do tipo PI (Proporcional Integral). A flexibilidade efetiva, obtida após a implementação da estrutura de controle é avaliada, e possíveis pontos críticos são adicionados e o projeto é refeito. Por fim, através da geração de modelos dinâmicos e projeto dos controladores, o desempenho do projeto pode ser checado.

Abstract

In this work it was developed a computational framework for synthesis of flexible and controllable Heat Exchanger Network. The synthesis was accomplished based on the superstructure proposed in the literature for minimizing simultaneously the operating cost and the investment cost. The general assumptions used by this formulation were discussed. It was assumed uncertainty in the inlet temperatures and flowrates. The framework for flexible design is based on the termed two stage strategy. The first stage is prior to the operation (design phase) where the design variables are chosen, i.e. the existence and dimension of the equipments. At the second stage (operation phase) the control variables are adjusted during operation on the realizations of the uncertain parameters. The design stage was accomplished with a multiperiod optimization problem resulting in a MINLP formulation. In order to exploit the block diagonal structure of multiperiod problems, a decomposition technique based on the concept of Lagrangean Relaxation was developed as an alternative in order to solve the formulation for large scale problems. The operation stage checks whether the design selected in the previous step is able to operate over the space of uncertain parameters. This step was assessed by the Flexibility Index evaluation through a MI(N)LP formulation using the Active set strategy. If the design is sufficient flexible the procedure terminates; otherwise, the critical point obtained from the flexibility evaluation is included in the current set of periods, and a new multiperiod problem is solved in order to obtain a new design. Once the flexible design is achieved a MILP model is solved in order to define the control structure selection according to controllability metrics, i.e. the set of manipulated inputs (taken from the general set of potential manipulations) that can ensure the outlet temperatures target using standard feedback controllers, e.g. PID controllers. The effective flexibility is evaluated in order to check if the design is feasible for the given control structure selection, otherwise a new critical point is identified and the multiperiod design is performed again. Later on, the dynamic model and closed loop performance can be checked.

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CSS	Control Structure Selection
FI	Flexibility Index
HEN	Heat Exchanger Network
HEN	Heat Exchanger Network
HENS	Heat Exchanger Network Synthesis
LP	Linear Programming
LD	Lagrangean Decomposition
LMTD	Logarithmic Mean Temperature Difference
MILP	Mixed Integer Linear Programming
MINLP	Mixed Integer Non Linear Programming
NLP	Non Linear Programming
PI	Controle de ação proporcional e integral
PID	Controle de ação proporcional, integral e derivativa
RGA	Matriz de ganho relativo
TAC	Total Annual Cost
TSS	Two Stage Strategy

Capítulo 1

Introdução

Os processos industriais demandam de grandes quantidades de energia para o seu funcionamento e manutenção das condições operacionais especificadas no projeto. Do ponto de vista energético, um processo industrial pode ser visto como três componentes integrados: (*i*) o *processo industrial* propriamente dito, constituído principalmente de unidades de reação, separação e reciclo; (*ii*) o *sistema de utilidades* que fornece para o processo recursos externos, tais como, ar, combustíveis fósseis, vapor, água, dentre outros; e (*iii*) o *sistema de recuperação de calor*, onde as correntes de processo são integradas através da síntese de uma rede de transferência de calor de forma a melhorar a eficiência energética do processo reduzindo o consumo de utilidades e os impactos ambientais inerentes a utilização e/ou geração desses recursos-vide Figura 1.1 (Aaltola, 2003).

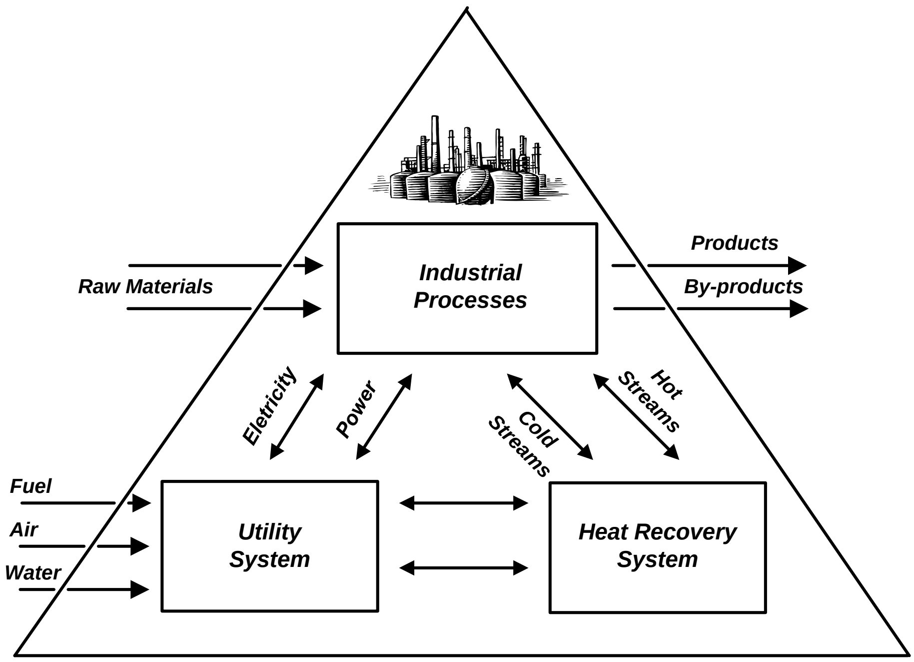

Figura 1.1: Sistema geral de processo.

Durante a operação algumas correntes de processo devem ser aquecidas enquanto que outras devem ser resfriadas para satisfazer as condições operacionais. O alcance dessas condições é sempre possível através de uma solução trivial, onde todas as correntes de processo são conduzidas de suas temperaturas de entrada para suas respectivas temperaturas de saída utilizando recursos externos, ou seja, utilidades quentes e frias provenientes do sistema de utilidades. No entanto, esta não é uma solução interessante do ponto de visto econômico ou ambiental, uma vez que nenhuma energia é recuperada. Correntes de processo que apresentam necessidades ou disponibilidades energéticas, podem se suprir mutuamente através de um trocador de calor, desde que mantida a factibilidade termodinâmica do sistema. O residual energético é então suprido pelas chamadas utilidades. As trocas de energia internas geram a chamada Rede de Trocadores de Calor (*HEN-Heat Exchanger Network*), que pode ser vista como a forma sistemática através da qual se torna possível a integração energética do processo. A solução desejada, ou seja, a rede final com o arranjo entre os trocadores e correntes de processo é aquela com mínimo custo total anual (*TAC-Total Annual Cost*) decorrente do custo de investimento em trocadores de calor e do custo operacional inerente ao consumo de utilidades. O projeto de uma rede de trocadores de calor envolve grande parcela do custo operacional e de investimento de um processo como um todo, sendo seu projeto um fator chave para um processo economicamente viável.

O projeto de uma HEN é usualmente conduzido em estado estacionário, para uma condição operacional fixa. É assumido que um sistema de controle possa ser projetado para manter o processo operando dentro das especificações. O esforço total de projeto (em nível de sistema) requerido para uma HEN tipicamente envolve três estágios (Glemmstad, 1997):

- *Projeto Nominal*. Uma ou mais HENs são sintetizadas para uma dada condição operacional, usando técnicas apropriadas;

- *Análise de Flexibilidade e Controlabilidade*. As redes são investigadas no que diz respeito a sua flexibilidade e controlabilidade, e possivelmente algumas modificações são realizadas (ex. aumento de área, modificações estruturais);

- *Operação*. Um sistema de controle é projetado de forma apropriada, envolvendo a seleção da estrutura de controle, projeto de controladores e possivelmente algum método de otimização online usando os graus de liberdade adicionais.

Para cada passo, alguma rede pode ser rejeitada ou o projetista deve retroceder ao passo anterior para encontrar outras alternativas. Atualmente, esses passos são realizados de forma sequencial, e quando um sistema de controle simples não pode ser implementado, ou a rede deve ser reprojetada ou deve-se tolerar que o processo pode não preencher todos os requerimentos operacionais, de flexibilidade e controlabilidade.

Embora HENs seja um dos problemas de síntese mais extensivamente estudados na literatura, considerações operacionais têm sido largamente negligenciadas. Existe um espaço aberto para pesquisa com o objetivo de incorporar na síntese além dos aspectos econômicos e ambientais, a operabilidade do mesmo. Ainda, diversas ferramentas têm sido desenvolvidas para síntese de uma rede para o ponto nominal, no entanto, o número de trabalhos que leva em consideração aspectos operacionais, principalmente controlabilidade, ainda é bastante reduzido.

1.1 Projeto Nominal

O problema da síntese de redes de transferência de calor tem recebido uma atenção considerável na literatura nas últimas décadas (ver Gundersen e Naes (1988); e Furman e Sahinidis (2002) como extensas revisões sobre o assunto). O problema básico de síntese de redes pode ser sentenciado da seguinte maneira (Furman e Sahinidis, 2001):

Dado um conjunto de correntes quentes que precisam ser resfriadas, um conjunto de correntes frias que precisam ser aquecidas, ambas de sua temperatura de entrada até sua temperatura de saída, para uma dada vazão e uma estimativa para os coeficientes de transferência de calor de cada corrente; um conjunto de utilidades disponíveis, desenvolva uma rede de trocadores, isto é a configuração entre os trocadores os calor de calor que resulte no mínimo custo total em base anualizada resultante do custo de investimento em equipamentos associado ao custo operacional em termos de consumo de utilidades.

Duas grandes escolas se desenvolveram nas últimas décadas: (*i*) uma primeira que utiliza métodos termodinâmicos associados a regras heurísticas (Linnhoff e Hindmarsh, 1983); (*ii*) e uma segunda que utiliza métodos de programação matemática linear, e não-linear inteira mista, utilizando superestruturas (Ciric, Floudas e Grossmann, 1986; Ciric e Floudas; 1991; e Yee e Grossmann, 1990). A primeira escola deu origem a uma tecnologia de aplicação simples e bastante difundida a nível industrial conhecida como Tecnologia "*Pinch*" (tecnologia do ponto de estrangulamento). A sua aplicação permite a fácil identificação de melhorias e possibilidades de integração. No entanto, a síntese da rede é manual e requer um grande conhecimento do processo por parte do projetista. Na programação matemática a síntese é automática e são facilmente incorporadas restrições operacionais, devido ao tratamento matemático do problema. No entanto, esta técnica apresenta a desvantagem de resultar em problemas relativamente mais complexos e de difícil solução devido a sua natureza combinatorial e as não convexidades inerentes aos modelos não lineares que descrevem cada unidade e suas respectivas dimensões. A menos que técnicas especializadas de otimização global sejam utilizadas, apenas soluções subótimas, isto é mínimos locais, são encontradas.

1.2 Operabilidade: Flexibilidade e Controlabilidade

Embora a integração de processos seja primordialmente motivada por benefícios econômicos e aspectos ambientais, uma possível desvantagem em sua utilização consiste no fato de que o processo integrado pode ser mais difícil de operar e manter controle do mesmo. Esta característica pode ser limitante na aplicação em um processo industrial real. A rede introduz interações mudando o comportamento estático e dinâmico do processo. Em um processo integrado, distúrbios ou variáveis manipuladas podem não somente prover efeitos locais, mas estes efeitos podem se espalhar para grande parte da planta. Um projeto puramente baseado em aspectos econômicos pode conduzir a eliminação de configurações que sejam mais facilmente controladas, embora ligeiramente menos econômicas, em favor de projetos mais econômicos que podem ser extremamente difíceis de controlar. Em um projeto passível de implementação, é importante uma estratégia para operação e controle que resulte em nível razoável de desempenho dinâmico e boa capacidade de rejeição de distúrbios.

De maneira geral, o termo operabilidade inclui todos os aspectos relacionados à operação de um processo tais como, flexibilidade, segurança, confiabilidade, controlabilidade, partidas e paradas etc. Neste trabalho o termo operabilidade terá a sua dimensão limitada a flexibilidade e controlabilidade, estando relacionado com a facilidade de se operar o processo em condições normais não envolvendo falhas e nem paradas ou partidas de unidades. Enquanto que flexibilidade é um conceito associado ao comportamento estacionário do processo, a controlabilidade leva aspectos dinâmicos em consideração.

1.2.1 Flexibilidade

Um pré-requisito para operabilidade é que a HEN seja suficientemente flexível, isto é, tenha habilidade de manter a operação sujeita a incertezas (variações) nas condições operacionais enquanto satisfaz as especificações em estado estacionário. Essas variações são usualmente referidas como incertezas e são intrínsecas ao processo. Uma rede capaz de operar sujeita a incerteza é então dita flexível. A incerteza pode ser descrita através de variações esperadas, tendo como referência os valores nominais. Define-se então uma região de incerteza para a qual se deseja que a rede tenha operação factível. Para HENs, são geralmente assumidos variações (incertezas) nas temperaturas de entrada e vazões.

O termo flexibilidade estrutural se refere a flexibilidade de uma dada rede quando o diferencial de temperatura nos terminais dos trocadores de calor são permitidos assumir valores nulos, isto é, as áreas dos trocadores podem ser infinitamente grandes. A flexibilidade real é limitada pelas áreas instaladas dos trocadores e será menor que a flexibilidade estrutural. Durante uma análise de flexibilidade assume-se que um conjunto de variáveis podem ser ajustadas livremente durante a operação. É importante estar ciente que a flexibilidade da rede pode ser limitada pela estratégia de controle utilizada. Mesmo que uma análise de flexibilidade indique que uma rede suficientemente flexível, não se tem nenhuma garantia que a estratégia de controle empregada irá ajustar as variáveis manipuladas de tal forma que a flexibilidade total seja mantida. Na literatura, este ponto parece ter sido negligenciado, ou tem sido implicitamente assumido que a estratégia de controle não irá deteriorar a flexibilidade. Enquanto que a flexibilidade é uma propriedade do "*design*", a Flexibilidade Efetiva consiste na habilidade de uma rede controlada de manter a operação factível sujeito a incerteza, sendo uma propriedade do design e da estratégia de controle.

1.2.2 Controle e Controlabilidade

O principal objetivo de controle em uma HEN consiste em garantir que as temperaturas de saída das correntes participantes da rede sejam mantidas, seja em um valor fixo (*setpoint*), ou dentro de uma faixa (*range*). Em alguns casos, outros objetivos podem ser estabelecidos, tais como: manutenção da carga térmica de condensadores e refervedores numa coluna de destilação que estejam integrados à rede, ou alguma temperatura interna, por questões de segurança ou mesmo para prevenir a decomposição. Ainda, podem existir temperaturas de saída sem nenhuma especificação, ou apenas limitadas por valores limites (máximo ou mínimo).

Durante a operação, graus de liberdade ou variáveis manipuladas são necessárias para o controle e otimização. Diferentes possibilidades são ilustradas na Figura 1.2: 1- Vazões ou cargas térmicas de utilidades; 2-Frações de *bypass*; 3- Frações de *split*; 4- vazões da própria corrente de processo; 5- Área do trocador (e.g. condensador inundado); 6- Vazão de reciclo (e.g. se o *fouling* do trocador de calor é reduzido por aumento da vazão).

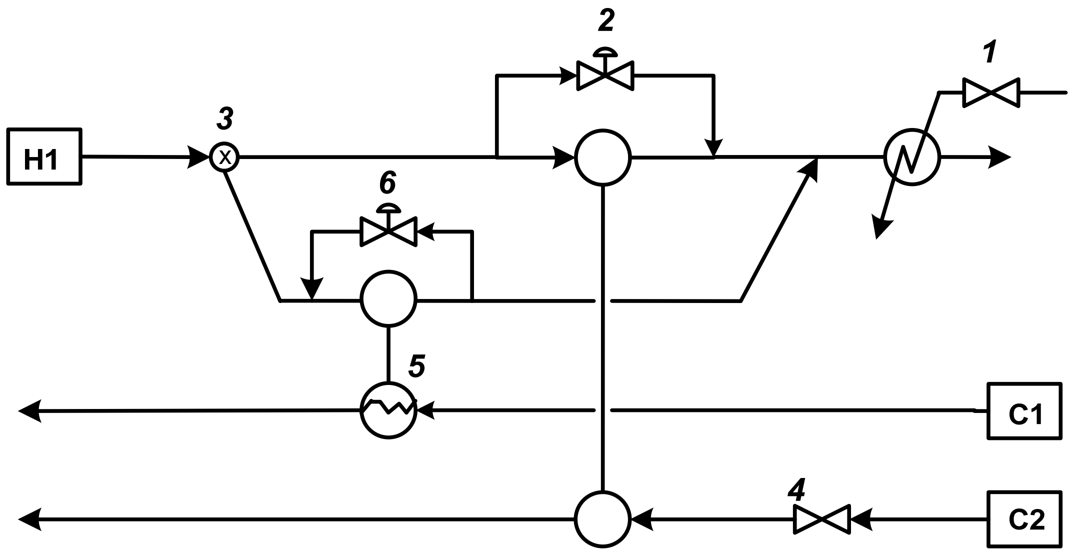

Figura 1.2: Possíveis variáveis manipuladas em HENs.

A configuração da rede pode impor limitações no sistema de controle, tais como (i) zeros no semi-plano direito; (ii) atrasos; e (iii) interações entre as malhas de controle. Morari (1992) apontou que a controlabilidade de uma rede é altamente dependente de sua configuração. O termo controlabilidade é usualmente utilizado, simplesmente significando o quão fácil o processo é de se controlar. Nesse contexto, a controlabilidade é uma característica inerente ao processo e independente do projeto do controlador.

Neste trabalho é assumido que a rede seja controlada através de um projeto de controle descentralizado, uma vez que estes são bastante utilizados na indústria e preferíveis frente a estruturas centralizadas, devido à sua simplicidade e facilidade na manutenção e operação. Diversas métricas de controlabilidade são disponíveis na literatura, e.g. RGA (Britsol, 1966), número de condicionamento mínimo, dentre outras, que embora independam da sintonia do controlador, dependem da seleção da estrutura de controle, ou seja, do emparelhamento usado variável controlada-manipulada. Uma descrição compreensível de análise de controlabilidade é apresentada em Skogestad e Postlewaite (1996) e Trierweiler (1997).

1.3 Operação Ótima

Durante a operação, ao contrário da fase de "*design*", os compromissos entre custo operacional e de investimento são completamente irrelevantes, uma vez que a estrutura encontra-se definida, assim como as áreas dos trocadores. A única questão importante consiste em como explorar a configuração de forma mais eficiente possível. Para uma HEN com dada estrutura, áreas dos trocadores de calor, coeficientes de transferência de calor e temperaturas de entrada e saída, a operação ótima é alcançada se (Glemmstad, 1997):

- as temperaturas de saída são mantidas em estado estacionário (objetivo principal);
- o custo de utilidades é minimizado (objetivo secundário);
- e o comportamento dinâmico é satisfatório (objetivo terciário).

O objetivo secundário requer a existência de graus de liberdade adicionais, enquanto que manipulações selecionadas de um conjunto potencial são dedicadas ao objetivo principal. O terceiro objetivo é um pouco mais vago. Embora seja possível a definição de especificações rigorosas no comportamento dinâmico, em um consenso, é desejável que a rede controlada seja estável e que o comportamento dinâmico seja necessariamente não oscilatório ou lento. Com esta definição de operação ótima, onde os dois primeiros objetivos se aplicam ao estado estacionário, é claramente assumido que o processo seja operado próximo ao estacionário na maior parte do tempo, de forma que o custo operacional total seja dominado pelo desempenho no estado estacionário, e não pelo estado transiente.

1.4 Objetivos

O principal objetivo deste trabalho consiste no desenvolvimento de uma metodologia computacional que seja capaz de levar em consideração aspectos operacionais como flexibilidade e controlabilidade ainda na etapa de projeto. É desejável que o método desenvolvido seja uma abordagem sistemática passível de aplicação em problemas de escala industrial, com o auxílio das ferramentas computacionais e "*solvers*" disponíveis comercialmente. O problema básico estudado neste trabalho pode ser sentenciado da seguinte maneira:

Dados, (i) as correntes de processos e de utilidades disponíveis, com suas respectivas temperaturas, vazões e estimativa dos coeficientes de transferência de calor; (ii) um range especificado para as incertezas (distúrbios), ou seja, variações esperadas para as temperaturas de entrada e vazões, para o qual a flexibilidade da configuração é desejada; (iii) um diferencial mínimo de temperatura admissível nos trocadores de calor (ΔT_{min}); (iv) um conjunto de variáveis controladas, e (v) um conjunto de potenciais manipuladas, do qual um subconjunto deve ser selecionado pela estrutura de controle (emparelhamento). Encontre a configuração com: (i) mínimo custo total anual (custo de investimento e operacional); (ii) que seja capaz de operar de forma factível sujeito ao range de distúrbio especificado; (iii) que seja efetivamente flexível uma vez implementado um sistema de controle descentralizado, cuja estrutura de controle é selecionada através da minimização de critérios de controlabilidade; (iv) por fim, cujo comportamento dinâmico seja satisfatório.

Este consiste em um problema desafiador, principalmente devido à sua natureza combinatorial e à sua não convexidade decorrente da não linearidade do tipo bilinear associada à multiplicação da vazão com a temperatura envolvidas nos modelos matemáticos.

1.5 O Escopo da Pesquisa

Este trabalho considera essencialmente *grassroots designs* (projetos novos), e seu caráter multidisciplinar envolve as seguintes áreas: (i) síntese de redes de transferência de calor; (ii) análise de factibilidade e flexibilidade; (iii) análise de controlabilidade; (iv) operação ótima de redes de trocadores de calor; (v) projeto de processos flexíveis, ou seja, sujeitos a incerteza; (vi) seleção de estrutura de controle (emparelhamento) em problemas combinatoriais; e (vii) síntese simultânea de processos flexíveis e controláveis. Uma visão geral e esquemática do desenvolvimento deste trabalho é apresentada na Figura 1.3.

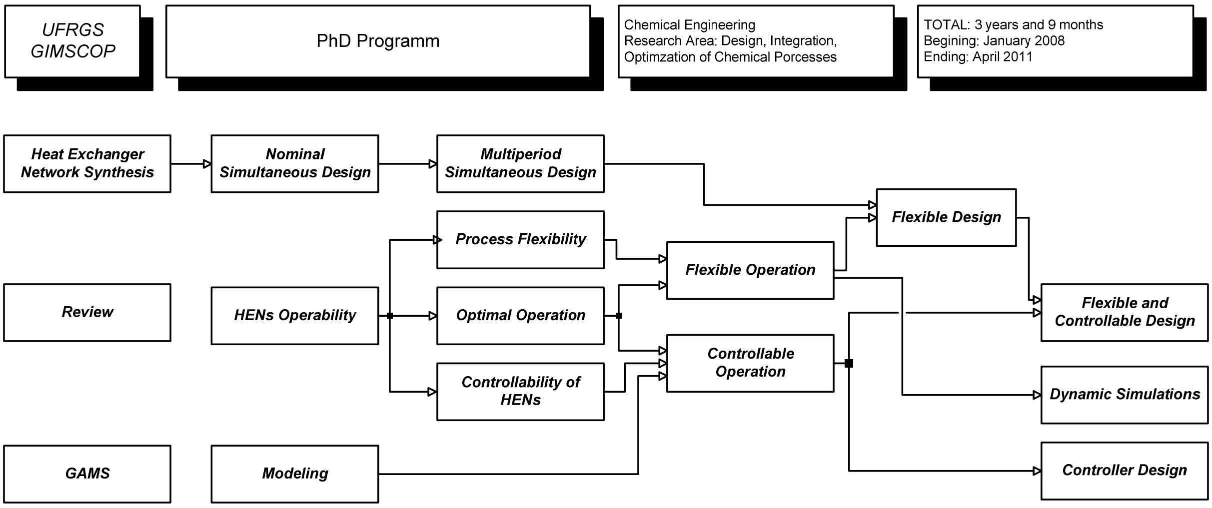

Figura 1.3: Visão esquemática e sequencial dos módulos de desenvolvimento do trabalho.

As seguintes considerações gerais são inerentes a esse trabalho: (i) propriedades físicas constantes; (ii) não ocorrência de mudança de fase; (iii) modo de operação contracorrente nos trocadores de calor; (iv) geometria de trocadores de calor casco e tubo; (v) perda de carga negligenciada bem como outras considerações fluidodinâmicas; (vi) não ocorrência de *fouling*; (vii) *bypasses* podem ser alocados em torno dos trocadores de calor; ($viii$) vazões de utilidades, frações de *split* e frações de *bypass* podem ser ajustadas durante a operação (ix) hipótese de controle perfeito durante a análise de flexibilidade, isto é, manipulações podem ser ajustadas para compensar os parâmetros incertos e nenhum atraso nas medições, ou ajustes são consideradas; (x) limitações são impostas a flexibilidade pela estrutura de controle; (xi) temperaturas de saída como variáveis controladas; e (xii) temperaturas de entrada e vazões de capacidade calorífica como parâmetros incertos (distúrbios). Considerações adicionais são explicitamente realizadas diretamente no corpo do texto quando pertinente.

1.6 Estruturação do Trabalho

Neste capítulo foi apresentada uma visão geral do trabalho, bem como sua motivação, principais objetivos e considerações realizadas. No Capítulo 2 é apresenta uma revisão bibliográfica sobre o assunto, tanto para a síntese de redes na forma como ela é realizada convencionalmente, como é apresentado o que já existe na literatura no que diz respeito a flexibilidade de controlabilidade no projeto de redes de trocadores de calor.

A partir daí essa tese foi estruturada na forma de artigos científicos. No Capítulo 3 é realizado um estudo comparativo entre os principais métodos baseados em programação matemática existente para o projeto nominal. Estes foram implementados no sistema de modelagem e otimização GAMS. Foram desenvolvidos estratégias para inicialização dos problemas de otimização, sem as quais não seria possível obtenção das soluções. Foi realizada uma comparação sistemática entre os métodos e os "*solvers*" disponíveis. Optou-se por utilizar o modelo SYNHEAT (Yee e Grossmann, 1990) como base para o desenvolvimento deste trabalho. No Capítulo 4, as principais características deste modelo são avaliadas através de uma comparação com outro modelo confeccionado, baseado na mesma superestrutura mas sem as hipóteses simplificadoras do modelo SYNHEAT.

No Capítulo 5, são apresentadas diferentes extensões multiperíodo baseadas no modelo SYNHEAT, onde cada período corresponde a uma condição operacional. Adicionalmente, a estrutura do modelo foi explorada através da proposição de uma técnica de decomposição baseada em relaxação Lagrangeana associado a regras heurísticas. O problema multiperíodo com N períodos é decomposto em N subproblemas, possibilitando a solução para problemas de grande escala.

No Capítulo 6, um procedimento computacional através de um esquema iterativo em dois estágios é apresentado para o projeto de redes flexíveis. Para cada estágio, diferentes propostas são apresentadas e exemplos numéricos ilustram a eficácia do procedimento como método sistemático para geração de redes flexíveis.

No Capítulo 7, o projeto do sistema de controle é incorporado no procedimento em dois estágios apresentado no Capítulo 6, bem como a avaliação da flexibilidade efetiva após a implementação do sistema de controle resultando na proposta final deste trabalho para geração de redes que sejam flexíveis e controláveis com uma simples estrutura de controle descentralizada utilizando controladores do tipo PID.

O Capítulo 8 apresenta as principais conclusões relativas ao trabalho, além das principais considerações e contribuições. Ainda, são apresentadas sugestões para trabalho futuros visando a extensão deste trabalho e sua aplicabilidade em nível industrial.

Este trabalho é complementado por alguns Apêndices. No Apêndice A é apresentada a modelagem estática e dinâmica dos componentes presentes nas redes, possibilitando o desenvolvimento de uma geração sistemática para o modelo da rede a partir dos modelos de cada componente. Esses modelos são utilizados nas simulações e na seleção da estrutura de controle. No Apêndice B, são anexados dois estudos relativos à operabilidade de redes. Inicialmente é feito um estudo comparativo entre diferentes projetos em termos de flexibilidade, posteriormente o projeto da estrutura de controle é analisado e é proposta uma metodologia para o projeto do sistema de controle para uma dada estrutura. Neste momento o projeto foi considerado fixo e as áreas são reprojetadas de acordo com a necessidade de rejeição a distúrbios. Por fim, no Apêndice C, uma revisão geral sobre métodos matemáticos que foram utilizados nesse trabalho é apresentada.

1.7 Produção Técnica e Contribuições

Os diversos capítulos que fazem parte desta tese serão (ou já foram) publicados em revistas científicas e congressos internacionais, as quais são a seguir listadas:

Capítulo 3: Escobar and Trierweiler (2009). Optimal Heat Exchanger Network Synthesis: Initialization Strategies and Systematic Comparison. *Submetido para a revista internacional Industrial & Engineering Chemistry Research*. *Este trabalho foi apresentado no VII Oktoberfórum em Porto Alegre-Brazil, Outubro 21-23, 2008.*

Capítulo 4: Escobar, Trierweiler and Grossmann (2010). Mixed-Integer Nonlinear Programming Models for Optimal Simultaneous Synthesis of Heat Exchangers Network. *Publicado no website (minlp.org), consistindo de uma biblioteca virtual de modelos MINLP*[1] *apresentando uma descrição de problemas,modelagem e dicussão.*

Capítulo 5: Escobar, Trierweiler and Grossmann (2011). A Lagrangean Heuristic Approach for Multiperiod Heat Exchanger Network Synthesis. *Em revisão para ser submetido para a revista internacional Computers & Chemical Engineering. Este trabalho foi também apresentado na reunião anual do CAPD (CAPD Annual Meeting) em Pittsburgh, em Março 8-10 de 2010.*

Capítulo 6: Escobar, Trierweiler and Grossmann (2011). Simultaneous Synthesis of Flexible Heat Exchanger Networks. *Apresentado no European Symposium on Computer Aided Process Engineering (ESCAPE) 21 na Grécia, em Maio/Junho de 2011. Este trabalho foi também apresentado no IX Oktoberfórum em Porto Alegre-Brazil, em Outubro 19-21 de 2010.*

Capítulo 7: Escobar, Trierweiler and Grossmann (2011). Simultaneous Synthesis of Flexible and Controllable Heat Exchanger Network. *Em revisão para ser submetido para a revista internacional Computers & Chemical Engineering. Este trabalho foi também apresentado na forma de Seminário (PSE Seminar) na Carnegie Mellon University em Pittsburgh-USA, no dia 30 de Agosto de 2010.*

Apêndice B: Parte I Escobar and Trierweiler (2009). Operational Flexibility of Heat Exchanger Networks. *Artigo apresentado no congresso International Symposium on Advanced Control of Chemical Processes (ADCHEM 2009) em Istanbul, Turkia, em Julho 12-15 de 2009.* **Parte II:** Escobar and Trierweiler (2010). Operational Controllability of Heat Exchanger Networks. *Artigo apresentado no congresso 9th International Symposium on Dynamics and Control of Process Systems (DYCOPS) em Leuven, Belgica, 5-7 Julho de 2010. Uma versão preliminar desse estudo foi apresentado no congresso 10th International Symposium on Process Systems Engineering (PSE'09) em Salvador,Brazil em Agosto 16-20 de 2009.*

Avaliação de Índice de Flexibilidade para HENs: Foram desenvolvidos exemplos de avaliação de índice de flexibilidade utilizando diferentes técnicas publicado no *Newton interfaces* (interface interativa de problemas MINLP) disponível online[2] e utilizada com fins didáticos na disciplina Advanced Process System Engineering ministrada pelo professor Ignácio Grossmann na Carnegie Mellon University.

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[1] http://www.minlp.org/

[2] http://newton.cheme.cmu.edu/interfaces/flexnet/main.html

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Capítulo 2

O Estado da Arte em HENS

2.1 Síntese de Redes de Transferência de Calor

O projeto de Redes de Transferência de Calor (HENS) é um dos problemas de síntese mais estudados em processos industriais, estando intimamente relacionado com a eficiência energética do processo. Furman e Sahinidis (2002) reportaram mais de 400 artigos publicados sobre o assunto ao longo dos últimos 40 anos. Desde a primeira grande crise energética a nível mundial, na década de 70, os engenheiros de processo têm investido significativos esforços no sentido de desenvolver metodologias sistemáticas orientadas para a máxima recuperação de energia dentro do próprio processo. Estes estudos levaram ao rápido desenvolvimento de uma nova área, conhecida como Integração de Processos. A Integração de Processos consiste em uma forma eficiente de a indústria aumentar sua produtividade através da redução no consumo de energia, água e matéria-prima, redução em emissões de gases e na geração de rejeitos. Com esta tecnologia é possível reduzir significativamente o custo operacional de plantas existentes, enquanto os novos processos podem ser projetados com redução nos custos operacionais e de investimento.

As primeiras abordagens durante os anos 60 e inicio dos anos 70 trataram o problema da síntese como uma tarefa única. As principais técnicas propostas apresentaram limitações na teoria e nos algoritmos de otimização disponíveis, que foram o gargalo na expansão e aplicabilidade de técnicas de programação matemática naquele momento (Floudas, 1995). O trabalho de Hohman (1971), que recebeu pouco reconhecimento nos anos 70 e o trabalho de Linnhoff e Flower (1978a; 1978b) introduziram o conceito de temperatura "*pinch*". Como resultado, a ênfase da pesquisa mudou para decomposição do problema original em três subproblemas (*targets*): (i) mínimo custo de utilidades; (ii) mínimo numero de trocadores de calor; e (iii) mínimo custo de investimento. A principal vantagem na decomposição do problema consiste no fato de os subproblemas poderem ser tratados de maneira mais simples se comparado ao problema sem decomposição.

Nesta abordagem, os seguintes subproblemas são tratados sequencialmente:

i. Mínimo consumo de utilidades, correspondendo à máxima recuperação de energia em uma rede viável termodinamicamente para um dado ΔT_{min}; parâmetro de projeto que estabelece o compromisso entre o custo operacional e de investimento. O problema de determinação do mínimo consumo de utilidades foi primeiro introduzido por Hohmann (1971) e Linnhoff e Flower (1978) através de métodos gráficos, e posteriormente como um problema de programação linear LP (*Linear Programming*), através do modelo LP *transportation* por Cerda et al. (1983), e mais comumente o modelo LP *transshipment* de Papoulias e Grossmann (1983);

ii. Mínimo número de unidades, que determina o número de trocadores, a combinação entre as correntes e a distribuição de carga térmica para um consumo fixo de utilidades determinado na etapa anterior. O modelo MILP (*Mixed Integer Linear Programming*) *transportation* de Cerda e Westerberg (1983) e o modelo MILP *transshipment* de Papoulias e Grossamnn (1983) são os mais difundidos;

iii. Mínimo custo de investimento baseado na distribuição de carga térmica, e no consumo de utilidades determinado nas etapas anteriores. Usando uma formulação baseada em superestrutura, desenvolvida por Floudas et al. (1986), um problema de programação não linear (NLP) é formulado para minimização do custo total da rede. A função objetivo consiste na minimização do custo de investimento sujeito aos balanços de massa, balanços de energia e equação de projeto envolvendo média logarítmica de temperatura. Devido ao produto "vazão x temperatura" inserido pelos balanços a formulação é não convexa, o que significa que o uso de solvers convencionais (e.g. CONOPT e MINOS) resultam em mínimos locais (Floudas e Ciric, 1989).

A Tecnologia Pinch foi consolidada no trabalho de Linnhoff e Hindmarsh (1983), tendo grande aceitação pelas indústrias, principalmente devido a sua facilidade de aplicação. Uma das principais vantagens desta técnica consiste na determinação do potencial de integração a frente do projeto. Por outro lado, uma vez identificado potencial de integração, a síntese da rede segue um conjunto de regras heurísticas, sendo tediosa sua aplicação de forma sistemática em problemas de larga escala. Os métodos de decomposição, ou sequenciais, seja pela Tecnologia Pinch ou por programação matemática tem provado em muitos estudos de caso ser uma ferramenta poderosa para síntese de redes de transferência de calor. A principal vantagem nesse tipo de abordagem consiste na facilidade de sua aplicação. No entanto, apresentam como principal desvantagem o fato de que os compromissos entre consumo de energia, e investimento em unidades e áreas não são considerados de forma rigorosa podendo resultar em redes subótimas (Floudas, 1995).

Devido às limitações apresentadas pelos métodos sequenciais, a pesquisa no final dos anos 80 e inicio dos anos 90 teve foco na resolução do problema da síntese como um único problema, considerando a minimização de todos os compromissos entre custo de investimento e custo operacional simultaneamente. Esta abordagem normalmente resulta em formulações MINLPs (*Mixed Integer Non Linear Programming*) cuja solução provê o consumo de utilidades, o número de unidades e sua respectiva carga térmica, as áreas dos trocadores de calor e a topologia da rede com mínimo custo total anual simultaneamente.

Floudas e Ciric (1989) propuseram a resolução da combinação das correntes e a configuração da rede ao mesmo tempo, usando a superestrutura apresentada em Floudas et al. (1986). Neste problema, o consumo de utilidades é fixo, sendo previamente determinado pelo modelo LP *transshipment* de Papoulias e Grossmann (1983). Posteriormente, Ciric e Floudas (1991) propuseram uma abordagem sem nenhuma decomposição. A formulação matemática é bastante similar à anterior, mas o consumo de utilidade é tratado como variável desconhecida, sendo os compromissos minimizados simultaneamente.

Yee e Grossmann (1990) propuseram uma abordagem alternativa ao método simultâneo de Ciric e Floudas (1991). Eles postularam uma superestrutura baseada em estágios de troca térmica e assumiram a hipótese de mistura isotérmica em cada estágio, gerando um modelo simplificado popularmente conhecido como SYNHEAT. A principal motivação por trás desse estudo foi de desenvolver um modelo matemático cujas restrições sejam todas lineares, de forma que as não linearidades aparecem somente na função objetivo. Apesar da eliminação do espaço de busca de um número considerável de estruturas, Yee e Grossmann (1990) demonstraram em seu trabalho que boas HENs, do ponto de vista econômico, podem ser obtidas usando este modelo.

Na Figura 2.1 é apresentada uma visão geral e cronológica das principais abordagens apresentadas. Em suma, nos anos 70 a Tecnologia Pinch foi fundamentada, sendo consolidada apenas no ano de 1983. Em paralelo, métodos sequenciais foram desenvolvidos nos anos 80; e finalmente, no inicio dos anos 90, abordagens simultâneas foram propostas.

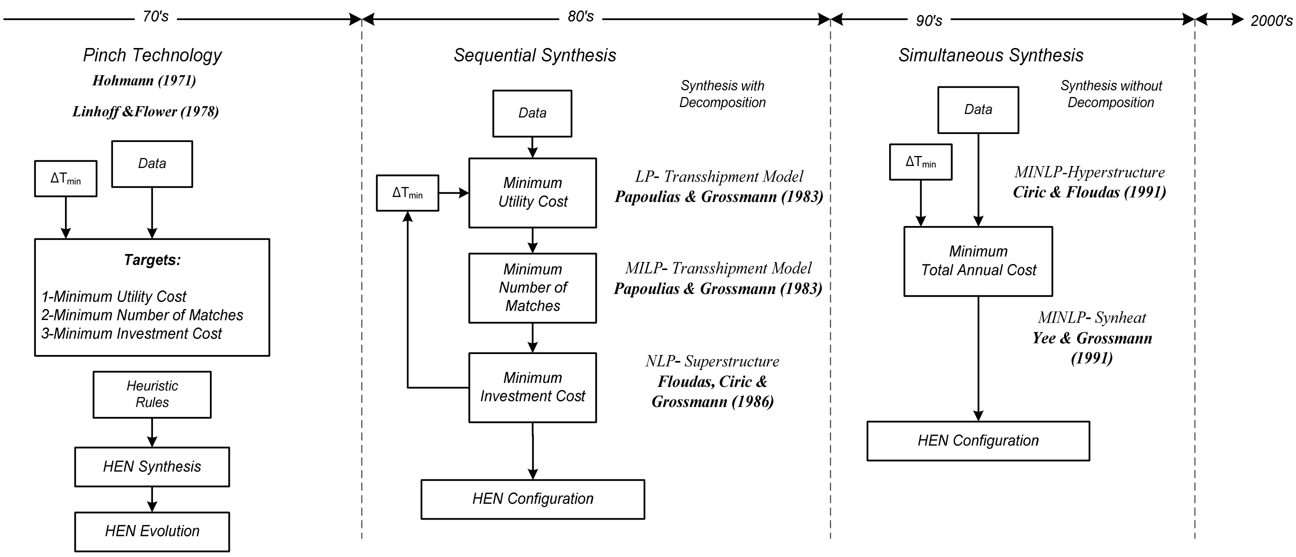

Figura 2.1: Panorama histórico das principais abordagens para HENS.

2.2 Flexibilidade de HENs

Diversos autores têm desenvolvido métodos sistemáticos para síntese de redes de transferência de calor (HENS) sujeito a incerteza, ou seja, redes que sejam flexíveis. De maneira geral a incerteza é descrita a partir da especificação de limites inferiores e superiores para cada parâmetro incerto, gerando uma região descrita por um hiperretângulo no espaço de parâmetros incertos. Uma visão geral dos trabalhos mais notáveis nessa área é apresentada na Figura 2.2.

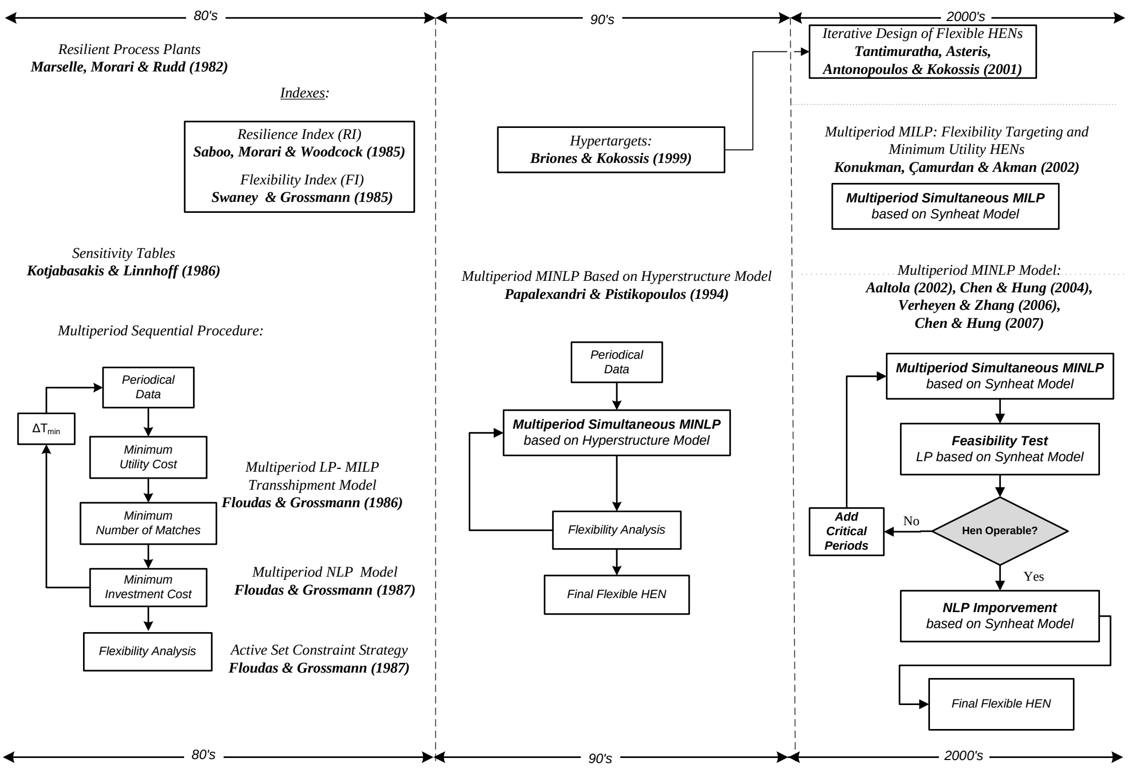

Figura 2.2: Visão geral de métodos para síntese de redes flexíveis

O trabalho de Marselle et al. (1982) é considerado na literatura como pioneiro em considerações operacionais em HENs. Neste trabalho foi desenvolvido o conceito de HENs resilientes, que podem tolerar incertezas nas temperaturas de entrada e vazões das correntes. A metodologia proposta de projeto, no entanto, necessita uma combinação manual de projetos em diferentes cenários considerados críticos para a operação, tornando a aplicação deste método para problemas em larga escala praticamente impossível.

Com o intuito de mensurar o grau de flexibilidade de uma HEN, Saboo et al., (1985) propuseram o Índice de Resiliência (RI). Este índice caracteriza a máxima incerteza total que uma rede pode tolerar enquanto permanece viável. Desta forma o RI pode ser usado como métrica comparativa entre diferentes configurações. Swaney e Grossmann (1985) introduziram o Índice de Flexibilidade (FI), que representa o máximo desvio de um parâmetro incerto enquanto ainda permanece dentro da região viável. Esse índice é baseado na região esperada de operação, assumindo valor maior ou igual à unidade quando toda região esperada de operação está contida dentro da região viável, e menor do que um caso contrário. Naquele momento, os algoritmos propostos para o seu calculo se basearam em considerações que tornavam o problema tratável apenas para o caso em que as restrições fossem convexas.

Kotjabasakis e Linnhoff (1986) introduziram o conceito de tabelas de sensibilidade para o projeto de redes flexíveis. Foi desenvolvida uma metodologia com intuito de encontrar qual trocador deve ter sua área aumentada e qual deve ser "bypassado" para tornar um dado projeto flexível, dado um conjunto de cenários operacionais.

Grossmann e Floudas (1987) introduziram a estratégia do conjunto ativo (*active set strategy*) para automação na solução do Índice de Flexibilidade. Este método foi desenvolvido com o intuito de sobrepor a limitação anterior, e o modelo resultante MI(N)LP pode ser usado para o caso geral com restrições não convexas.

Tantimuratha et al., (2000) propuseram um procedimento em dois estágios, onde o primeiro estágio consiste em utilizar o modelo *hypertarget* desenvolvido previamente por Brione e Kokossis (1999) para seleção da combinação entre as correntes e, num segundo momento, o custo total anual é minimizado. Este método, no entanto, pode ainda conduzir a soluções subótimas, uma vez que se basea em decomposição.

2.2.1 Abordagens Multiperíodo

Para um dado "*design*" sujeito a incerteza, não se sabe a condição operacional que o processo se encontra submetido durante a operação. Este problema pode ser tratado na programação matemática através de uma modelagem estocástica, onde é minimizado o valor esperado da função custo. No entanto, pode-se formular uma aproximação determinística se um conjunto de cenários (ou períodos) forem postulados e o problema de projeto for estendido para representação multiperíodo. Diferentes abordagens multiperíodos foram propostas na literatura para HENs.

Floudas e Grossmann (1987a, 1987b) propuseram um método sequencial que combina a extensão multiperíodo do modelo (MILP) *transshipment* com a estratégia do conjunto ativo (*active set strategy*) para projetar redes com um determinado grau de flexibilidade. O método foi aplicado com sucesso em diferentes estudos de caso. Papalexandri e Pistikopoulos (1994) apresentaram uma metodologia para síntese e retrofit (redesign) de redes que sejam flexíveis e estruturalmente controláveis usando um problema MINLP. A extensão multiperíodo foi baseada na superestrutura de Floudas et al. (1986) envolvendo um grande número de restrições não convexas, limitando sua aplicabilidade em problemas relativamente pequenos. De acordo com Mathisen (1994), a formulação proposta resulta em um modelo muito complexo cuja solução apresentada para exemplos simples não foram convincentes. Aparentemente esta linha de pesquisa não apresentou uma continuidade.

Desenvolvimentos mais recentes nesta área foram realizados baseados no modelo SYNHEAT de Yee e Grossmann (1990). A característica de que a região de busca deste modelo é linear o torna bastante robusto e de fácil utilização, possibilitando a obtenção de boas soluções utilizando os algoritmos disponíveis para solução de MINLPs. Konukman et al. (2002) propuseram uma formulação multiperíodo no qual as áreas de troca térmicas não são consideradas explicitamente, sendo apenas limitadas por restrições nas forças motrizes, reduzindo o problema a um MILP. Esta formulação presume que região viável no espaço de parâmetros incertos é convexa; portanto a solução ótima é explorada tendo como base os vértices da região de incerteza. Isto limita a aplicação para o projeto com incertezas presentes apenas nas temperaturas de entrada. A formulação é então resolvida sucessivamente para diferentes metas de flexibilidade, com o objetivo de revelar a necessidade de modificações estruturais e seus correspondentes consumos de utilidades.

Aaltola (2003) propôs uma formulação MINLP baseada no modelo SYNHEAT considerando todos os compromissos simultaneamente. No modelo proposto, *bypasses* não foram modelados explicitamente, o que iria introduzir não linearidades no conjunto de restrições. Para representar o efeito do *bypass*, a área é permitida variar em diferentes cenários. Desta forma, cada cenário apresenta uma área de troca térmica requerida, considerando que a máxima área corresponde à área que deve ser instalada, uma vez que as outras condições operacionais podem ser obtidas através da instalação de um *bypass*. O ponto chave neste trabalho consiste no fato de que não se sabe *a priori* para qual cenário a máxima área vai ocorrer. Visando sobrepor essa escolha discreta, Aaltola considerou a área instalada como a média das áreas requeridas, o que claramente resulta em um subestimativa da área instalada e, portanto uma subestimativa do custo de investimento. Essa abordagem foi inserida em um procedimento em dois estágios, sendo o "*design*" realizado no primeiro estágio através da solução do problema multiperíodo. Num segundo estágio, a operação é verificada através de um problema multiperíodo linear (LP), onde cada período é obtido a partir de uma densa discretização da região de incerteza. Vale mencionar que a viabilidade nos períodos não garante que o projeto seja viável entre eles.

Chen e Hung (2004) propuseram uma formulação MINLP multiperíodo baseada no modelo SYNHEAT. Com o intuito de evitar a subestimativa do custo de investimento, eles propuseram introduzir a função "*max*" no modelo, resultando em um modelo cuja função objetivo é não diferenciável e consequentemente mais cara do ponto de vista computacional. Como metodologia para geração de redes flexíveis, eles associaram o multiperíodo proposto ao cálculo do índice de flexibilidade usando a estratégia do conjunto ativo e a adição de cortes inteiros para evitar o retorno da mesma estrutura. No entanto, esta formulação requer uma derivação manual das condições de otimalidade (condições de KKT), levando uma metodologia aplicável apenas a estudos de casos pequenos, bem como os que foram ilustrados nesse trabalho.

Verheyen e Zhang (2006) propuseram uma modificação do modelo MINLP de Aaltola, no qual o cálculo das áreas máximas é encontrado pela adição de inequações não lineares no conjunto de restrições resultando em formulação rigorosa, na qual o custo de investimento é calculado de forma exata. Essas restrições adicionais impõe que a área seja maior ou igual à área requerida em cada período, e a direção da função objetivo garante que essa restrição esteja ativa pelo menos para o pior caso, onde a área máxima ocorre. Neste trabalho, diferentes estudos de caso foram usados para comparar os dois modelos. A principal conclusão é de que os modelos eram equivalentes, sendo encontrada uma diferença máxima de 5 % .

Chen e Hung (2007) propuseram uma metodologia para redes flexíveis, associando o modelo proposto por Verheyen e Zhang (2006) com um teste de viabilidade multiperiodo do tipo LP onde os cenários são gerados randomicamente dentro da região de incerteza. Se todos os pontos forem concluídos viáveis, a rede é considerada flexível. Caso contrário, o ponto crítico (ponto de máxima violação das restrições) é adicionado ao conjunto de períodos e o modelo multiperíodo é resolvido novamente. Uma vez encontrada a rede flexível, a configuração é fixa, fixando as variáveis binárias do problema e o MINLP se reduz a um NLP, no qual balanços de energia adicionais são impostos ao modelo de forma a remover a consideração de mistura isotérmica.

2.3 *Controle* e Controlabilidade de HENs

No trabalho de Marselle et al. (1982), uma vez gerado o projeto flexível, foi proposta uma metodologia baseada em teoria de grafos para a seleção da estrutura de controle. Calandranis e Stephanopoulos (1986) propuseram uma análise de operabilidade baseado apenas na informação estrutural, onde os parâmetros incertos são considerados como distúrbios. As características estruturais da rede são usadas para identificar rotas para alocação de cargas térmicas para sorvedouros disponíveis e para desenvolvimento de um controlador inteligente para seleção das melhores rotas.

Kotjabasakis e Linnhoff (1986) propuseram um método evolucionário, usando o conceito de "*downstream paths*" e tabelas de sensibilidade. A principal contribuição deste trabalho foi a conceito de "*downstream paths*", definido como uma conexão não quebrada entre as variáveis de entrada e de saída. Distúrbios se propagam através das redes somente se existe um "*downstream path*" entre o distúrbio e as saídas da rede. A ausência de "*downstream paths*" resulta em uma singularidade estrutural. Foram propostas três alternativas para proteger uma variável controlada de ser afetada por um distúrbio: (i) quebrando downstream paths, ou (ii) inserção de elementos a montante, ou (iii) adicão de *bypasses*.

Georgiou e Floudas (1990) exploraram o conceito de singularidade estrutural para propor uma metodologia que considera simultaneamente o projeto da rede que apresente controlabilidade estrutural. Eles incorporam as condições de rejeição a distúrbios na formulação na superestrutura. A resolução do MINLP resultante conduz a um projeto com mínimo custo e que é capaz de rejeitar distúrbios. Os exemplos ilustrados mostram distúrbios em apenas um ou duas correntes, e apenas um subconjunto das temperaturas de saídas como variáveis controladas. Variáveis binárias são utilizadas para indicar a existência de *downstream paths*, restrições adicionais garantem a inexistência de um "*downstream path*" dos distúrbios para as variáveis controladas. É bastante evidente que se todas as correntes apresentam distúrbios, esta metodologia favorece o projeto de uma rede sem integração energética.

Huang e Fan (1992) propuseram uma estratégia distribuída para projetar redes que são economicamente efetivas e altamente controláveis em termos de rejeição de distúrbios. Eles construíram uma tabela de controlabilidade baseada na classificação da informação do processo, tais como intensidade do distúrbio e precisão do controle. A partir desta tabela várias regras heurísticas são propostas de acordo com os objetivos de controle.

Papalexandri e Pistikopoulos (1994 a, b) desenvolveram um modelo simultâneo para o projeto de redes flexíveis e estruturalmente controlável. Foi utilizado um MINLP baseado na superestrutura de Ciric e Floudas (1991) considerando uma modelagem explícita de *bypass*. Eles utilizaram o conceito de controlabilidade estrutural defino por Morari e Stephanopoulos (1980) baseado no "*rank*" genérico da matriz de representação estrutural do problema.

Mathisen (1994) investigou de forma bastante compreensível o projeto e o controle de HENs e propuseram a formulação de regras heurísticas. Estas regras são sentenciadas através de proposições lógicas que são então convertidas em inequeções lineares envolvendo variáveis binárias. Foi proposta a incorporação destas heurísticas numa formulação matemática para gerar rede com boa operabilidade.

Konukman et al. (1994) estudaram o efeito das correntes de *bypass* na propagação de distúrbios usando uma formulação não linear minimizando os desvios de temperaturas para um dado "*design*". Konukman et al. (1995) propuseram uma abordagem similar para projetar redes que sejam controláveis, considerando uma formulação multiperíodo para todos os possíveis predefinidos direções de estúrdios.

Yang et al. (1996) introduziram um modelo simplificado para rápida quantificação da propagação de um distúrbio em uma rede através da estimativa dos máximos desvios nas temperaturas de saída. Esse modelo apresenta então grande potencial para ser embutido dentro de um problema de síntese.

Glemmestad (1997) propôs uma metodologia para operação ótima de HENs para uma estrutura fixa. Uma contribuição importante deste trabalho foi uma análise de graus de liberdade que pode ser usada para checar se a operação pode ser otimizada, uma vez consumidos os graus de liberdade pela estrutura de controle. Foi também apresentado uma metodologia para operação ótima da rede baseado em uma otimização "*online*" para estado estacionário. Este procedimento requer que o modelo seja resolvido periodicamente durante a operação para seleção do emparelhamento adequado baseado em análise RGA (*Relative Gain Array*).

Uzturk e Akman (1997) descreveram um método para seleção da estrutura de controle usando alocação de "*bypasses*" via RGA e estruturas de controle centralizadas e descentralizadas. Diferentes configurações são então comparadas em termos de custo de índice de resiliência (RI).

Aguilera e Marchetti (1998) propuseram um método de controle e otimização online para HENs. Eles postularam que quando frações de *splits* não são usadas como variáveis manipuladas, mas apenas vazões de utilidades e frações de *bypass*, a operação ótima pode ser formulada com um problema LP. Esta foi a principal contribuição deste trabalho. Foi também discutido os graus de liberdade com respeito a otimização de HENs durante operação.

Oliveira (2001) propôs uma metodologia sequencial onde HENs são sintetizadas utilizando Tecnologia Pinch e a estrutura é então adaptada para um conjunto de cenários de distúrbios definidos previamente. Uma análise RGA e SVD é utilizada para seleção da estrutura de controle, e cujo desempenho é verificado a partir de simulação dinâmica.

Yan et al. (2001) desenvolveram um método iterativo baseado em modelo para o projeto de bypass para obtenção de redes controláveis. Em seu procedimento, o modelo de Yan et al. (1996) foi estendido para caracterizar não somente os distúrbios, mas também o efeito das potenciais variáveis manipuladas. O objetivo foi determinar deve ser "bypassado", a partir de uma análise RGA, e sua respectiva fração nominal determinada a partir do modelo.

Westphalen et al. (2003) propuseram um índice de controlabilidade (CI) para comparação de diferentes estruturas. O CI é definido como o menor número de condicionamento para todas as possíveis combinações de variáveis manipuladas.

Gonzales et al. (2006) propuseram uma estratégia de controle e otimização "*online*" para HENs através de um estrutura de controle em dois níveis. O nível regulatório com um controlador preditivo com restrições (MPC) e um nível supervisório composto de um otimizador "*online*". Este foi o único trabalho encontrado na literatura que relata o uso de controle preditivo para o controle de HENs.

Lersbamrungsuk et al. (2007) propuseram um procedimento sistemático para a obtenção da ótima operação de redes. Uma formulação linear envolvendo puramente variáveis binárias é resolvida para definir o emparelhamento numa estratégia de controle "*split-range*" e controle seletivo.

2.4 Quadro Comparativo

Pode-se perceber que a grande maioria dos trabalhos apresentados na literatura associa o projeto de controle com a ótima operação da rede, sendo desenvolvido sobre uma rede cuja topologia já tenha sido previamente projetada. Neste caso, possivelmente as áreas dos trocadores podem ser aumentadas permitindo uma maior capacidade de rejeição a distúrbios. Os poucos trabalhos que tentaram inserir a controlabilidade na etapa de projeto, usaram o conceito de controlabilidade estrutural, uma vez que esta é mais fácil de mensurar e é baseada apenas em informação estrutural. No presente trabalho, o termo controlabilidade, se refere à controlabilidade de entrada e saída dizendo respeito à facilidade de operação. A principal dificuldade encontrada consiste na sua quantificação durante a síntese uma vez que a estrutura e as condições operacionais não tenham sido determinadas, pois grande parte da teoria de controle se baseia em modelos linearizados em torno da condição operacional e para um projeto e "*layout*" fixo (Hovd e Skogestad, 1993). Uma revisão recente sobre métodos de seleção da estrutura de controle pode ser encontrada em Wal e Jager (2001), sendo que grande parte da pesquisa é voltada para utilização de métricas de controlabilidade. Na Tabela 2.1 é apresentado um quadro comparativo posicionando este trabalho em relação a trabalhos anteriores. Pode-se perceber a existência de trabalhos recentes para projeto de redes de trocadores de calor flexíveis, que sejam capazes de operar sujeita a variações nas vazões de temperaturas de entrada das correntes de processo. Apenas o trabalho de Papalexandri e Pistkopoulos (1994) leva em consideração no projeto da rede a controlabilidade estrutural, e não a controlabilidade de entrada e saída como proposto neste trabalho. Embora este seja um trabalho bastante reconhecido e citado na literatura, aparentemente não houve continuidade nessa linha de pesquisa, nem por parte de seus desenvolvedores, nem por possíveis seguidores. Avanços pouco significativos foram encontrados na literatura, embora a importância de se levar em consideração aspectos operacionais no projeto de um processo seja reconhecida nas últimas décadas.

Tabela 2.1: Pontos chaves dos desenvolvimentos anteriores comparado a este trabalho.

Work / *Item*	Floudas and Grossmann (1987)	Papalexandri and Pistikopoulos (1994)	Tantimuratha et al. (2001)	Konukman et al. (2002)	Aaltola (2002)	Chen and Hung (2004)	Verheyen and Zhang (2006)	Chen and Hung (2007)	This PhD work (2011)
Flexibility	×	×	×	×	×	×	×	×	×
Controllability		×							×
Temperature Variations	×	×	×	×	×	×	×	×	×
Flowrate Variations	×	×	×		×	×	×	×	×
Industrial Size Problems			×		×				×
Grassroot designs	×	×	×	×	×	×	×	×	×
Retrofit designs		×	×						
Simultaneously		×		×	×	×	×	×	×

Acrônimos

FI	*flexibility index*
HEN	*heat exchanger network*
$HENS$	*heat exchanger network synthesis*
$LMTD$	*log mean temperature difference*
LP	*linear programming*
$MILP$	*mixed integer linear programming*
$MINLP$	*mixed integer non linear programming*
NLP	*nonlinear programming*
RGA	*relative gain array*
RI	*resilience index*
SVD	*singular value decomposition*
TAC	*total annual cost*

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Chapter 3

Optimal Heat Exchanger Network Synthesis: Initialization Strategies and Systematic Comparison

Abstract:* *Heat Exchanger Network HEN is one of the most extensively studied synthesis/design problems in chemical engineering. This is attributed to the importance of determining energy costs and improving the energy recovery in chemical processes. Several synthesis procedures for heat exchanger networks have been published in the literature. However, only a modest number can be implemented as computer tools for the full automatic generation of network configurations. In spite of the computational methods evolution, some difficulties still need to be overcome, for example: computing time, and convergence problems. In this work, the main approaches to solve the problem of heat exchanger network synthesis were presented and were implemented using the General Algebraic Modeling System (GAMS) in a systematic way. In addition, initialization strategies for the nonlinear problems were proposed. Five case studies from literature with different dimensions are compared, analyzed, and discussed to show the main challenges involved by implementation and solution convergence.*

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Nomenclature

Abbreviations	
CC	*composite curve*
GCC	*grand composite curve*
$EMAT$	*exchanger minimum approach temperature*
HLD	*heat load distribution*
HEN	*heat exchanger network*
$HENS$	*heat exchanger network synthesis*
$HRAT$	*heat recovery approach temperature*
$LMTD$	*log mean temperature difference*
LP	*linear programming*
MER	*maximum energy recovery*
$MILP$	*mixed integer linear programming*
$MINLP$	*mixed integer non linear programming*
NLP	*nonlinear programming*
PDM	*pinch design method*
TAC	*total annual cost*

Sets	
CP	*set of cold process stream j*
CU	*set of cold utility*
HP	*set of hot process stream i*
HU	*set of hot utility*

Variables	*Units*	
$dt^1_{i,j}$	[ºC]	*temperature approach for the inlet for i and outlet for j in the exchanger for i and j*
$dt^2_{i,j}$	[ºC]	*temperature approach for the inlet for j and outlet for i in the exchanger for i and j*
$dt_{i,j,k}$	[ºC]	*temperature approach between hot stream i, cold stream j, at location k*
dt_{cui}	[ºC]	*temperature approach between hot stream i, and cold utility*
dt_{huj}	[ºC]	*temperature approach between cold stream j, and hot utility*
ΔT_1	[ºC]	*temperature approach in the terminal 1 of the heat exchanger*
ΔT_2	[ºC]	*temperature approach in the terminal 2 of the heat exchanger*
$f^{EH}_{i,j}$	[kW/K]	*hot flow capacity through the exchanger in the match i and j*
$f^{EC}_{i,j}$	[kW/K]	*cold flow capacity through the exchanger in the match i and j*
$f^{I}_{m,m'}$	[kW/K]	*flow capacity from initial splitter to the mixer preceding exchanger for m and m'*
$f^{E}_{m,m'}$	[kW/K]	*flow capacity through the exchanger in the match m and m'*
$f^{B}_{m,m',m''}$	[kW/K]	*flow capacity from splitter after the exchanger for m and m' to the mixer preceding exchanger for m and m''*
$f^{O}_{m,m'}$	[kW/K]	*flow capacity from splitter after the exchanger for m and m' to the final mixer*
$LMTD_{i,j}$	[ºC]	*log mean temperature difference between hot stream i and cold stream j*
$LMTD_{i,j,k}$	[ºC]	*log mean temperature difference between hot stream i, cold stream j, at stage k*

$LMTD_{cui}$	[°C]	*log mean temperature difference between hot stream i, and cold utility*
$LMTD_{huj}$	[°C]	*log mean temperature difference between cold stream j, and hot utility*
$Q_{i,j}$	[kW]	*heat load between hot stream i and cold stream j*
$Q_{i,j,k}$	[kW]	*heat load between hot stream i and cold stream j in temperature interval k*
Q^{CU}	[kW]	*minimum cold utility requirement*
Q^{HU}	[kW]	*minimum hot utility requirement*
$Q^{CU}_{j,k}$	[kW]	*heat load of cold utility j entering temperature interval k*
$Q^{HU}_{i,k}$	[kW]	*heat load of hot utility i entering temperature interval k*
$Q^{C}_{j,k}$	[kW]	*heat load of cold process stream j entering temperature interval k*
$Q^{H}_{i,k}$	[kW]	*heat load of hot process stream i entering temperature interval k*
$q_{i,j,k}$	[kW]	*heat load between hot stream i and cold stream j at stage k*
q_{cui}	[kW]	*heat load between hot stream i and cold utility*
q_{huj}	[kW]	*heat load between cold stream j and hot utility*
R_k	[kW]	*heat residual load out of temperature interval k*
$R_{i,k}$	[kW]	*heat residual of hot process stream/utility i out of temperature interval k*
$S_{i,j}$	[kW]	*auxiliary variable*
$T^{IH}_{i,j}$	[°C]	*inlet temperature of hot stream i to the exchanger for i and j*
$T^{OH}_{i,j}$	[°C]	*outlet temperature of hot stream i from the exchanger for i and j*
$T^{IC}_{i,j}$	[°C]	*inlet temperature of cold stream j to the exchanger for i and j*
$T^{OC}_{i,j}$	[°C]	*outlet temperature of cold stream j from the exchanger for i and j*
$T^{I}_{m,m'}$	[°C]	*inlet temperature to the exchanger for m and m'*
$T^{O}_{m,m'}$	[°C]	*outlet temperature to the exchanger for m and m'*
t^k_i	[°C]	*temperature of hot stream i at hot end of stage k*
t^k_j	[°C]	*temperature of cold stream j at hot end of stage k*
$xr^k_{i,j}$	-	*split ratio of flow capacity of hot stream i at stage k for the match i-j*
$yr^k_{i,j}$	-	*split ratio of flow capacity of cold stream j at stage k for the match i-j*

Binary Variables

$y_{i,j}$	-	*existence of the match between hot stream i and cold stream j*
$z_{i,j,k}$	-	*existence of the match between hot stream i, cold stream j, at stage k*
z_{cui}	-	*existence of the match between hot stream i, and cold utility*
z_{huj}	-	*existence of the match between cold stream j, and hot utility*

Parameters	*Units*	
α	-	*weight factor to the objective func. for min. number of matches*
γ	-	*weight factor to the objective func. for min. number of matches*

ε	-	*weigth factor to the objective func. for min. number of matches*
$\beta_{i,j}$	-	*exponent for the area cost in exchanger i -j*
Ccu_j	[$/kW.yr]	*utility cost coefficient for cooling utility j*
Chu_i	[$/kW.yr]	*utility cost coefficient for heating utility i*
$c_{i,j}$		*cost for heat math between hot stream i and cold stream j*
F_m	[kW/K]	*flow capacity of hot/cold stream m*
F_i	[kW/K]	*flow capacity of hot stream i*
F_j	[kW/K]	*flow capacity of cold stream j*
h_i	[kW/m^{2}K]	*heat transfer coefficient for hot stream i*
h_j	[kW/m^{2}K]	*heat transfer coefficient for cold stream j*
$Lb_{i,j}$	[kW]	*lower bound on the heat load between stream i and stream j*
$Q_{i,j}^V$	[kW]	*maximum vertical heat load between stream i and stream j*
$\Delta T_{i,j}^{max}$	[^{o}C]	*maximum possible temperature drop through exchanger i-j*
T_i^{in}	[^{o}C]	*inlet temperature of hot stream i*
T_j^{in}	[^{o}C]	*inlet temperature of hot stream i / cold stream j*
T_i^{out}	[^{o}C]	*outlet temperature of hot stream i / cold stream j*
T_j^{out}	[^{o}C]	*outlet temperature of cold stream j*
Ω	[kW]	*upper bound for heat exchangers*
Γ	[^{o}C]	*upper bound for temperature difference*
$U_{i,j}$	[kW/m^{2}K]	*overall heat transfer coefficient between hot stream i and cold stream j*
$Ub_{i,j}$	[kW]	*upper bound on the heat load between stream i and stream j*
$\omega_{i,j}$	-	*weights to the match i-j*

3.1 Introduction

Heat Exchanger Network Synthesis (HENS) has been the subject of a significant amount of research over the last 40 years. They represent one of the major components in a chemical processing system, because it is strongly related to the energy efficiency of the process. The heat exchanger network has the task of integrating the hot and the cold process streams in a process in order to reduce the amount of heating and cooling utilities that are required. The problem of synthesizing optimal network configurations has received considerable attention in the literature (see Gundersen and Naess, 1988; and Furman and Sahinidis, 2002, for good reviews).

The basic HENS problem can be stated as follows (Furman and Sahinidis, 2002):

Given a set of hot process streams HP, which should be cooled from its supply temperature to its target temperature; a set of cold process streams CP, which should be heated from its supply temperature to its target temperature; the heat capacities and flow rates of the hot and cold process streams; the utilities available (e.g., hot utilities HU and cold utilities CU) and their corresponding temperature and costs; develop a heat exchanger network with the minimum annualized investment and annual operating costs, i.e. minimum Total Annualized Cost (TAC).

Despite the great economic importance of HENS, it features a number of key difficulties (Floudas, 1995) that are associated with handling: (i) the potentially explosive combinatorial problem for identifying the best pairs of hot and cold streams so as enhance energy recovery; (ii) forbidden, required, and restricted matches; (iii) the optimal selection of the HEN structure; (iv) fixed and variable target temperatures; (v) temperature dependent physical and transport properties; (vi) different types of streams (e.g., liquid, vapor, and liquid-vapor); and (vii) different types of heat exchangers (e.g., counter-current, non counter-current, multi-stream), mixed materials of construction, and different pressure ratings.

The extensive research effort during the last decades toward addressing these aforementioned difficulties/issues exhibit variations in their objectives and solution approaches. The first approaches during 1960s and early 1970s treated the HEN synthesis problem as a single task. The main proposed techniques presented limitations on the theoretical and algorithmic aspects of optimization that were the bottleneck in expanding the applicability of the mathematical approaches that time (Floudas, 1995).

The work of Hohmann (1971), which received little recognition in the 1970s and the work of Linnhoff and Flower (1978a; 1978b) introduced the concept of the pinch point. As a result, the research emphasis shifted for decomposing the original problem into the three separate tasks: minimum utility cost, minimum number of matches, and minimum investment cost network. Furthermore, HEN synthesis approaches based on decomposition were developed via thermodynamic, heuristic, and optimization approaches.

The main advantage of HEN synthesis approaches based on decomposition into targets is that they involve simpler subproblems that can be treated in a much easier fashion than the original single-task problem. It is, however, this identical advantage that introduces a number of limitations. The main one is that the trade-offs between the utility consumption, the number of matches, the area requirement and the minimum investment cost are not take into account appropriately and may result in HEN designs that are suboptimal networks (Floudas, 1995).

Due to the limitations presented by the sequential HEN synthesis approaches, researches in the late 1980s and early 1990s focused on simultaneous approaches that attempt to treat the synthesis problem as a single-task problem considering, this way, all tradeoffs properly, and advances in theoretical and algorithmic aspects of optimization have allowed for important strides to be achieved via the optimization based approaches.

In Figure 3.1 a chronological overview of HEN approaches is presented. In 70’s the Pinch Technology was developed, which was adapted using in the mathematical programming in the 80’s by the sequential approach. Lastly, in the 90’s the simultaneous synthesis approach has been proposed.

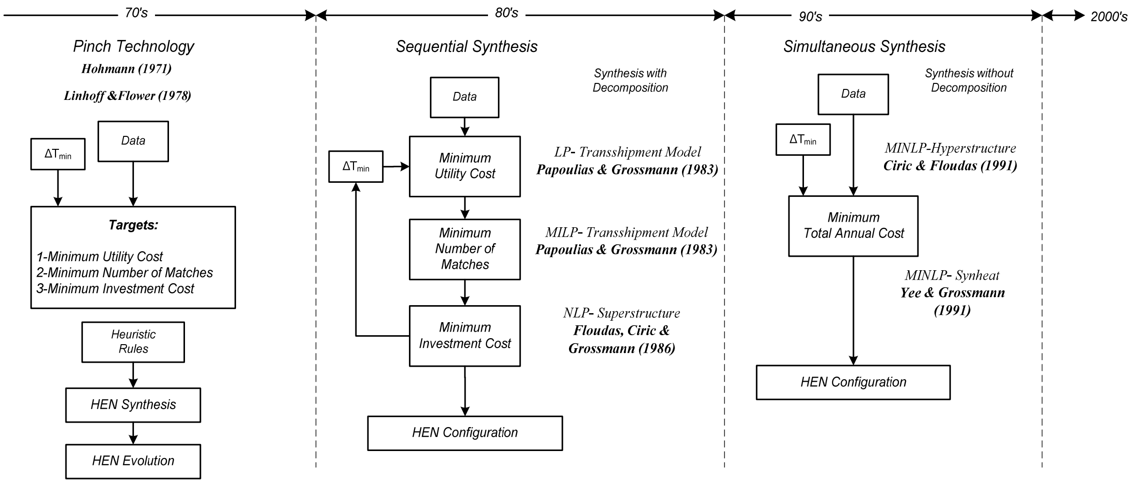

Figure 3.1: Historical panorama of HEN approaches over the last decades.

In the next section the main approaches available in the literature to handle the HENS are presented. The mathematical formulation is presented using a uniform notation, and all the problems were implemented in a systematic way using the GAMS modeling system. The Section 3.3 presents the strategy proposed to solve the different optimization problems. Five case studies with different dimensions are introduced in Section 3.4. The results are presented in the Section 3.5, where several HEN configurations have been synthesized based on different optimization approaches and different solvers. In this section the solvers are also systematically compared and some general recommendations and conclusions are also presented.

3.2 Approaches for Heat Exchanger Network

It is quite common to use some heuristic knowledge during the process design. It is particularly useful for Process Integration, which can combine heuristics with thermodynamic principles as done in the Pinch analysis and Exergy analysis. Hierarchical analysis and knowledge based systems are rule-based approaches with the ability to handle qualitative (or fuzzy) knowledge. Finally, optimization techniques can be divided into deterministic (Mathematical Programming) and non-deterministic methods (stochastic search methods such as Simulated Annealing and Genetic Algorithms).

An interesting classification of Process Integration methods (Gundersen, 2002) is to use the two-dimensional (automatic vs. interactive and quantitative vs. qualitative) representation shown in Figure 3.2. Hierarchical Analysis is placed in the middle of the figure to indicate that all sensible design methods are, or should be, based on this idea in order to make the complete design problem tractable by systematic methods.

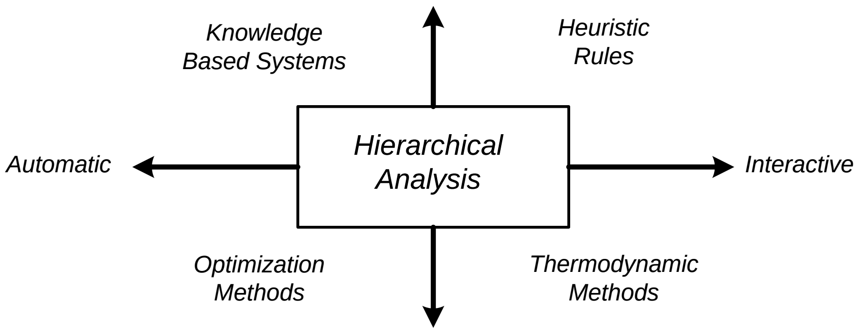

Figure 3.2: A possible Classification of Process Integration Methods.

3.2.1 Temperature Difference Definition

The design of any heat transfer equipment must always adhere to the second law of thermodynamics that prohibits any temperature crossover between the hot and the cold stream, i.e. a minimum heat transfer driving force must always be present for a feasible heat exchanger design. Thus the temperature of the hot and cold streams at any point in the exchanger must always have a minimum temperature difference (ΔT_{min}), and this value represents the bottleneck in the heat recovery.

At this point it is necessary to define and distinguish both temperatures approaches that are utilized at different stages of the HEN synthesis approaches. These are essentially parameters restrict the search space and hence simplify the problem. These parameters are defines as:

- ✓ $HRAT$, *heat recovery approach temperature*, is used to quantify utility consumption levels, and it is simply defined as the smallest vertical distance between the Composite Curves presented in next section; and

- ✓ ΔT_{min} or $EMAT$, *minimum approach temperature* specifies the minimum temperature difference between two streams exchanging heat within an exchanger.

In order to reach certain level of heat recovery (as specified by the $HRAT$), the temperatures approaches satisfy the relationship presented in (3.1).

$$HRAT \geq EMAT \tag{3.1}$$

The $HRAT$ parameterizes the utility consumption levels and it is usually equal to $EMAT$ in the strict pinch case, in which artificially do not allow for heat flow across the pinch and decompose the problem into subnetworks. The $EMAT$, however can in general be strictly smaller than $HRAT$ and this is denoted as the pseudo-pinch case, where heat is allowed to flow across the pinch point if the tradeoffs between the investment and the operating cost suggest it.

A very important step of the HEN synthesis approaches is the selection of these temperature approaches, since the tradeoffs involved (capital and energy costs) depends on these choice. The lower $HRAT$ chosen implies the lower the energy costs, but conversely the higher heat exchanger capital costs, as lower temperature driving forces in the network will result in the need for greater area. A large $HRAT$, on the other hand, will mean increased energy costs as there will be less overall heat recovery, but the required capital costs will be less. Therefore, this parameter has to be optimized, and it can have a great impact on the global solution.

3.2.2 Pinch Technology

Pinch Technology provides a systematic methodology for energy saving in processes and total sites. It is based on thermodynamic principles and heuristic rules. One of the main advantages of Pinch Technology over conventional design methods is the ability to set energy and capital cost targets for an individual process or for an entire production site ahead of the design. It has been successfully applied in many different industries, from petroleum and base chemicals to food and paper.

The term "Pinch Technology" was introduced by Linnhoff and Vredeveld (1984) to represent a new set of thermodynamically based methods that guarantee minimum energy levels in design of heat exchanger networks. The term Pinch Analysis is often used to represent the application of the tools and algorithms of Pinch Technology for studying industrial processes. The prime objective of pinch analysis is to achieve financial savings by better process heat integration.

In order to start the Pinch Analysis the necessary thermal data must be extracted from the process. This involves the identification of process heating and cooling duties. It is necessary to know the mass flowrates, specific heat capacity or heat of vaporization for streams with a phase change, supply and target temperatures of all streams that will possibly participate in the process integration analysis. This task is very important, and if not carried out properly, the final design will not be the best possible.

Pinch Analysis provides a target for the minimum energy consumption. The energy targets are obtained using a tool called the "$Composite\ Curves$" that consists of temperature-enthalpy (T-ΔH) profiles of cumulative heat availability in the process (the "hot composite curve") and cumulative heat demands in the process (the "cold composite curve") together in a graphical representation. The construction of the composite curves simply involves the addition of the enthalpy changes of the streams in the respective temperature intervals. The minimum energy target for the process is achieved by overlapping the hot and the cold composite curves, as shown in Figure 3.3, separating them by the $HRAT$ in the “pinch”, i.e. minimum driving force. This overlap shows the maximum process heat recovery possible, indicating that the remaining heating and cooling needs are the minimum hot utility requirement (Q^{HU}) and the minimum cold utility requirement (Q^{CU}) of the process for the chosen $HRAT$.

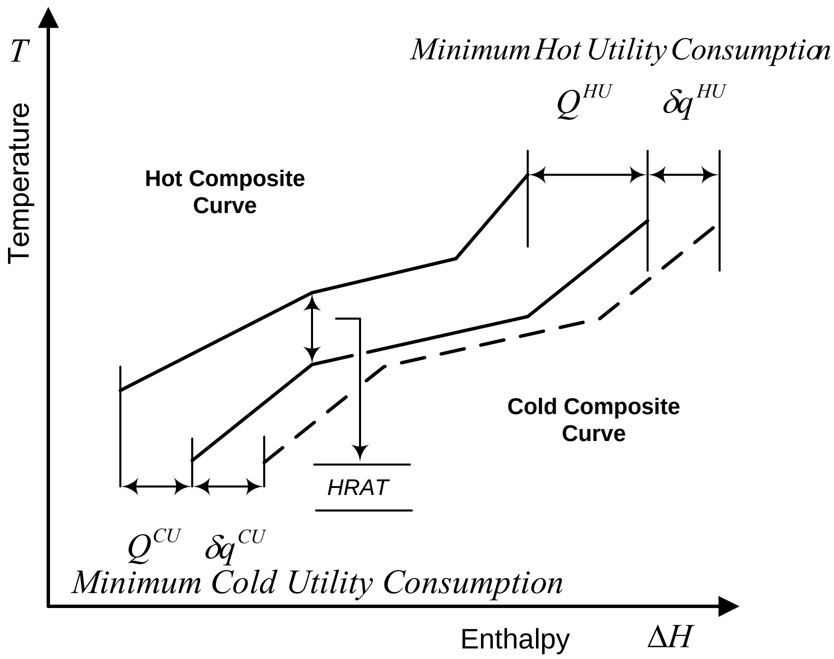

Figure 3.3: Composite curves and Pinch illustration.

Since we cannot bring the two composite curves closer (without violation of $HRAT$), the pinch point represents the bottleneck for further heat recovery. In fact, it partitions the temperature range into two subnetworks, one above the pinch, and one below the pinch. Heat flow cannot cross the pinch since the heat exchange driving forces is violated. Applying the first law of thermodynamics to each subnetwork is used to determine the minimum hot and cold utility requirements. The Pinch Technology, also, allows a visual representation for setting loads for the multiple utility levels. For this purpose, the $Grand\ Composite\ Curve$ is used (Linnhoff and Hindmarsh, 1983).

Despite the composite curves are excellent tools for learning the methods and understanding the overall energy situation, minimum energy consumption and the heat recovery level are more often obtained by numerical procedures. Typically, these are based on the $Heat\ Cascade$, where the supply and target temperatures of all process streams divide the temperature scale into temperature intervals, in the same way as the construction of the $Composite\ Curves$. In the $Heat\ Cascade$ different scales for the hot and cold temperatures are used. They differ by $HRAT$ to consider that the heat balance performed in each temperature interval ensures feasible heat transfer according to an economic criterion. The objective is to allow heat surplus in one interval to cascade down to the next interval, i.e. in a lower temperature level, in order to maximize heat recovery. The heat deficit that cannot be supplied after the cascade comes from hot utilities, and the residual heat surplus must be removed from the cascade in this lower level by cold utilities. Using a minimum utility consumption, the pinch is identified at the lower bound temperature in the interval with no heat surplus or deficit.

Summarizing, Pinch Technology gives three rules that form the basis for practical network designs: no external heating below the pinch; no external cooling above the pinch; and no heat transfer across the pinch. Violating any of these rules will lead to cross-pinch heat transfer resulting in an increase in the energy requirement beyond the targets. These rules compose the basis for the network design procedure, which ensures that there is no cross pinch heat transfer. For retrofit applications the design procedure "corrects" the exchangers that are passing the heat across the pinch.

The composite curves make it possible to determine the energy targets for a given value of $HRAT$ and they can also be used to determine the minimum heat transfer area required to achieve the energy targets ahead the network design (Linnhoff and Hindmarsh, 1983). The area target (A_{min}) is based on the assumption that "vertical" heat exchange adopted between the hot and the cold composite curves across the whole enthalpy range. This vertical arrangement, which is equivalent to pure counter-current area within the overall network, has been found to give a minimum total surface area. For a case where the process streams have uniform heat transfer coefficients (h_i and h_j) this is rigorous. In a new design situation, where there are no existing exchangers, it should be possible to design a network that is close to these targets.

In order to estimate the area target, the composite curve is partitioned into enthalpy intervals in the kick points and the estimation can be performed as expressed in the equation (3.2) proposed by Townsend and Linnhoff (1984) that keep being well accepted by adepts of Pinch Analysis. In 1990, Ahmad proved the applicability of this theoretical relation. This equation has typical estimation errors around 25% (Townsend and Linnhoff, 1984) so it is recommended to use a factor correction to estimate the real area (A_{REAL}) given by:

$$A_{min} = \sum_{l=1}^{\substack{Enthalpy \\ Intervals}} \frac{1}{LMTD_l}\left(\sum_{i=1}^{nh}\frac{Q_{il}^H}{h_i} + \sum_{j=1}^{nc}\frac{Q_{jl}^C}{h_j}\right);\ A_{REAL} \approx \frac{5}{4}A_{min} \qquad (3.2)$$

In equation (3.2), Q_{il}^H and Q_{jl}^C are the heat load contribution of the $i\text{-}th$ hot stream process/ $j\text{-}th$ cold stream process in the $l\text{-}th$ enthalpy interval respectively; and the $LMTD_l$ is the logarithmic mean temperature difference in the interval. It is also possible to set a target for the minimum number of heat exchanger units in a process (U_{min}). The minimum number of heat exchange units depends fundamentally on the total number of process and utility streams (N) involved in heat exchange. This can also be determined *a priori* by using a simplified form of Euler's graph theorem, $U_{min} = N - 1$, (Hohmann, 1971) applied separately on each subnetwork.

The targets for the minimum surface area and the number of units (U_{min}) can be combined together with the heat exchanger cost law equations to generate the targets for heat exchanger network capital cost, all heat exchangers are considered with the same size. The capital cost target can be super-imposed on the energy cost targets to obtain the minimum total cost target for the network as shown in Figure 3.4.

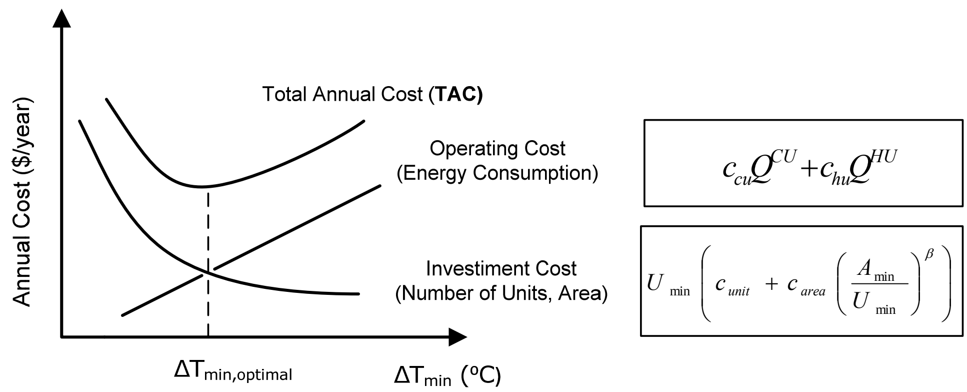

Figure 3.4: The trade-off between energy and capital costs for HENs.

The main purpose of estimating Total Annual Cost (TAC) is to identify a good starting point for network design selecting a value for $HRAT$. The Pinch Design Method (PDM) provides a strategy and matching rules that enable the engineer to obtain an initial network, which achieves the minimum energy target (Linnhoff and Hindmarsh, 1983). A stream grid is used as a drawing board in the design phase. The design is started at the pinch, where the driving forces are limited and the critical matches for maximum energy recovery must be selected, and develops by moving away from pinch.

The PDM with all rules can be found in Linnhoff and Hindmarsh (1983). Just to illustrate some rules, the number of cold streams above the pinch must be greater or equal than the number of hot streams; otherwise we have to split at least one cold stream to guarantee that it will be not necessary to use cold utilities above the pinch. Above the pinch the flow capacity of the cold stream must be greater than the flow capacity of the hot stream involved at the match to guarantee no $HRAT$ violation. Similar rules are used below the pinch

The main advantage of Pinch Technology against black box process optimization is the gained understanding of the process heat flows. On the other hand, Pinch analysis requires a lot of knowledge about the process. It is not quantitative handling with constraints and the network design is very interactive and tedious for large scale problems. However, it is very used because it is relatively easy make some significant improvement in the process.

3.2.3 Sequential Synthesis

One of the more prevalent methods for solving the HENS problem is the sequential synthesis method. This method involves partitioning the problem, usually by partitioning the temperature range of the problem into temperature intervals and possibly subnetworks, in accordance with a set of rules governing one of the pinch or pseudo-pinch design methods. The basic HENS problem is decomposed into three subproblems: (i) the minimum utilities cost; (ii) the minimum number of matches; and (iii) the minimum cost network problems. These problems are then solved according to the heuristic of finding the minimum cost network subject to the minimum number of units which is subject to the minimum utilities cost (Biegler, Grossmann, and Westerberg,1997).

The problem is usually partitioned into temperature intervals based on a minimum approach temperature (Linnhoff and Flower, 1978; Cerda, Westerberg, Mason, and Linnhoff, 1983; Biegler, Grossmann, and Westerberg, 1997) and sometimes enthalpy intervals as well (Gundersen and Grossmann, 1990; Gundersen, Duvold, and Hashemi-Ahmady, 1996). Also, the problem is sometimes divided into subnetworks based on the pinch point(s).

The most common problems used to solve for the minimum utilities cost, are the LP transshipment model of Papoulias and Grossmann (1983) and the LP transportation model of Cerda, Westerberg, Mason, and Linnhoff (1983). The minimum number of heat exchange matches and the heat load distribution based on the utility data of the previous step is usually determined by the MILP formulations of Papoulias and Grossmann (1983) and Cerda and Westerberg (1983). Another possibility it is to apply the vertical heat transfer formulations proposed by Gunderson and co-authors (Gundersen and Grossmann, 1990; Gundersen, Duvold, and Hashemi-Ahmady, 1996).

Finally, to derive a minimum cost network based on the matches and heat load information of the two previous steps, the superstructure-based formulation of Floudas, Ciric, and Grossmann (1986) is typically used. There are several implementations of sequential synthesis (Floudas, Ciric, and Grossmann, 1986; Saboo, Morari, and Colberg, 1986), but all of them preserve the same basic sequence outlined before and illustrated in Figure 3.1.

3.2.3.1 Minimum utility cost

The minimum utility cost problem of HENs can be stated as:

given a $HRAT$, and the process stream data, determine the minimum utility cost of a heat exchanger network without prior knowledge of the HEN configuration.

This is a very important target since it corresponds to the maximum energy recovery that can be attainable in a feasible HEN for a fixed $HRAT$. This target allows the elimination of several HEN structures which are not energy efficient and leads to near-optimal solutions as long as the energy is dominant cost item compared to the investment cost in the determining of Total Annualized Cost.

The key concept which allows for the determination of the minimum utility cost prior the knowing the HEN structure is the pinch point, presented in the section 3.2.2. As showed, a pinch point limits the maximum energy integration and hence is regarded thermodynamic bottleneck that prevents further energy integration whenever the feasibility constraints of heat exchange are violated. The minimum utility target cost in HENs can be formulated as a linear programming LP transshipment model (Papoulias and Grossmann, 1983), which corresponds to a well known model in process operation research (e.g., network problems), considering the intermediated nodes as temperature intervals, hot streams as sources and cold streams as destinations.

The procedure starts with the selection of $HRAT$ and the set of supply and targets temperatures of all processes streams are put on scale, shifting down the temperatures of the hot streams and shifting up the temperature of cold streams, both using $HRAT/2$. All set of temperatures are sorted to define temperature intervals between adjacent temperatures, where a heat balance can be performed as shown in Figure 3.5.

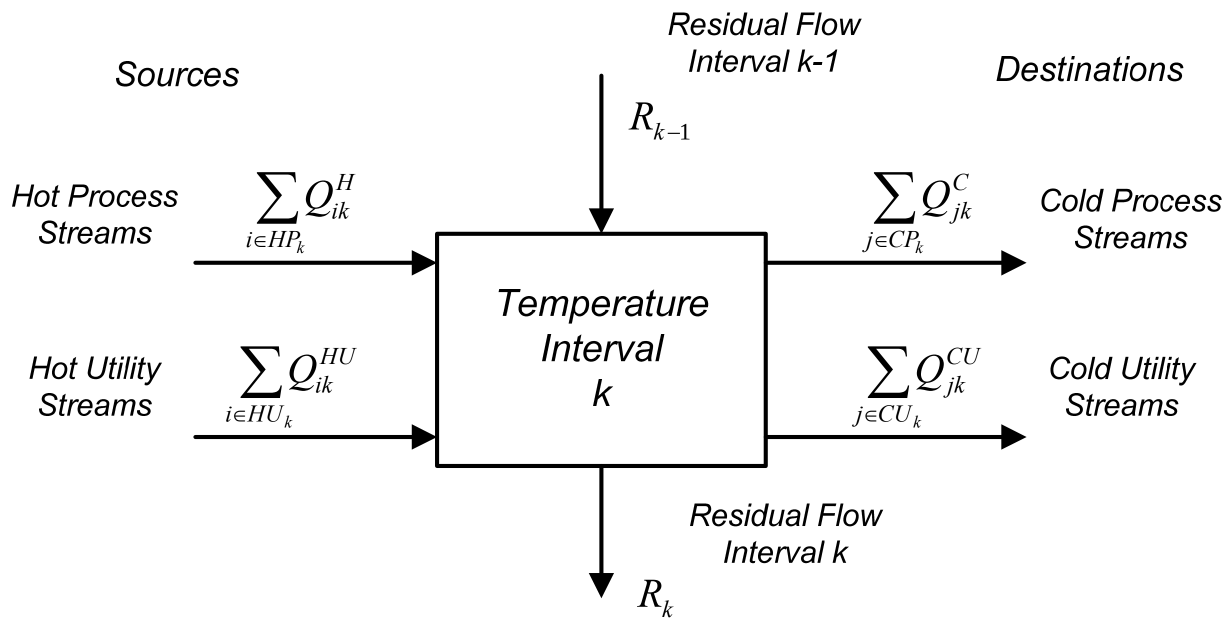

Figure 3.5: Heat Flow pattern of $k\text{-}th$ temperature interval.

Cerda et al. (1983) firstly proposed the transportation model for the calculation of the minimum utility cost, and subsequently Papoulias and Grossmann (1983) presented the transshipment model ($P1$) which requires fewer variables and constraints than the transportation model, and therefore, it is the most preferred implementation.

The solution of the LP transshipment model provides the required loads of hot and cold utility and the location of pinch point(s) if any. The pinch point(s) decompose the overall HEN into subproblems corresponding to above and below the pinch, if a single pinch point exists, or above the first pinch, between consecutive pinch point(s) and below the bottom pinch point, if multiple pinch points exist. These subproblems are denoted as subnetworks. It is the existence of pinch points that allows these subnetworks to be treated independently, with the implicit assumption that heat cannot cross the pinch point is not violated.

Problem P1: LP Transshipment Model (Papoulias and Grossmann, 1983).

Minimum Utility Cost

$$min \ \sum_{k}\sum_{j} Ccu_j Q_{j,k}^{CU} + \sum_{k}\sum_{i} Chu_i Q_{i,k}^{HU} \quad (F1)$$

subject to

Energy Balance of the k-th temperature interval

$$R_k - R_{k-1} + \sum_{j\in CU_k} Q_{j,k}^{CU} - \sum_{i\in HU_k} Q_{i,k}^{HU} = \sum_{i\in HP_k} Q_{i,k}^{H} - \sum_{j\in CP_k} Q_{j,k}^{C}$$

Nonnegative Constraints

$$Q_{j,k}^{CU} \geq 0; \quad Q_{i,k}^{HU} \geq 0; \quad R_k \geq 0 \quad (C1)$$

Assignments

$$R_0 = R_k = 0$$

3.2.3.2 Minimum Number of Matches

A useful target postulated so as to distinguish among the many HENs that satisfy the minimum utility cost is the minimum number of matches. The problem statement is: given the information provided from the minimum utility cost targets (i.e., loads of hot and cold utilities, location of pinch points, and hence subnetworks), determine for each subnetwork the pairs of hot and cold process stream, pairs of hot utilities and cold process stream, pairs of cold utilities and hot process stream, as well as the heat load of each match. The implicit assumption in postulating this target is that HENs that satisfy it are usually close to an optimal or near optimal total annualized cost solution (Floudas, 1995).

Papoulias and Grossmann (1983) proposed an MILP transshipment model for the formulation of the minimum number of matches target ($P2$). This model can be applied to each subnetwork of the HEN problem or to overall network. The basic idea is to model explicitly the potential heat exchange between all pairs of streams, excluding hot to cold utilities, with respect to existence of each match, amount of heat load of them, and amount of residual of each heat process stream/utility. A graphical representation is presented in Figure 3.6.

The objective function is a linear summation of all binary variables y_{ij}'s and simply minimizes the number of potential matches. All the energy balances and the definition constraints are linear in the residuals and heat loads. The relations between the continuous and binary variables are also linear since L_{ij} and U_{ij} are parameters corresponding to lower and upper bounds, respectively, on the heat exchange of each match.

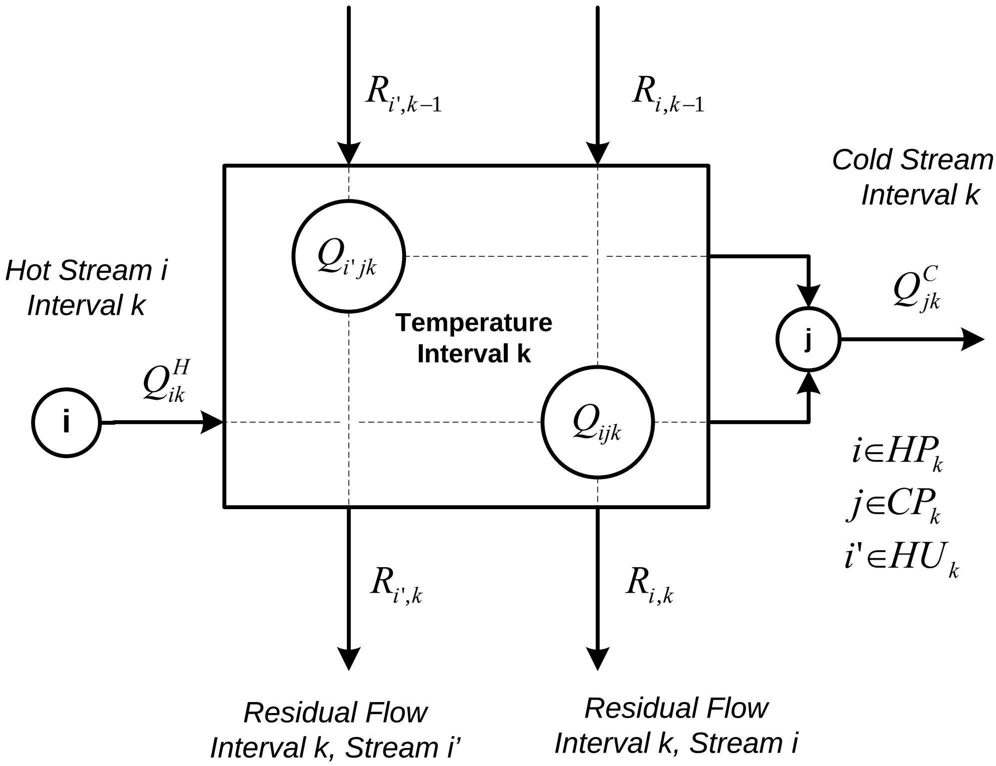

Figure 3.6: Graphical representation of temperature interval k for the MILP transshipment model.

It is important to understand the key role of these constraints, if y_{ij} assumes a unitary value, the heat load to that match can take place between the lower and the upper bound defined, on the other hand, if its value is zero the upper bound and the lower bound are equal to zero and hence the heat load is equal to zero as well, since the minimization of the objective function push the value towards this value.

The tightest bounds on the heat load of each potential match, for the case with no restriction on matches is given by:

$$Ub_{ij} = min\left\{\sum_k Q^H_{ik}, \sum_k Q^C_{jk}\right\}; \; Lb_{ij} = 0 \tag{3.3}$$

In case of required matches we can set the correspondent binary value to one, and in case of forbidden matches, set to zero. In addition, this formulation can deal with restricted heat loads on matches by the definition of the bounds, and also with preferred matches via assigning weights ω to each match in the objective function that becomes:

$$min \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} \omega_{ij} y_{ij} \tag{F2a}$$

Problem P2: MILP Transshipment Model (Papoulias and Grossmann, 1983).

Minimum Number of Matches

$$min \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} y_{ij} \quad \text{(F2)}$$

subject to

Energy Balance for each hot process stream and each interval k

$$R_{i,k} - R_{i,k-1} + \sum_{j \in CP_k \cup CU_k} Q_{ijk} = Q^H_{ik}\ , i \in HP_k$$

Energy Balance for each hot utility and each interval k

$$R_{i,k} - R_{i,k-1} + \sum_{j \in CP_k} Q_{ijk} = Q^H_{ik}\ , i \in HU_k$$

Energy Balance for each cold process stream and each interval k

$$\sum_{i \in HP_k \cup HU_k} Q_{ijk} = Q^C_{jk}\ , j \in CP_k \quad \text{(C2a)}$$

Energy Balance for each cold utility and each interval k

$$\sum_{j \in HP_k} Q_{ijk} = Q^C_{jk}\ , j \in CU_k$$

Definitions of total residual flows at each interval

$$R_k - \sum_{i \in HP_k \cup HU_k} R_{ik} = 0$$

Definitions of heat loads of each match

$$Q_{ij} = \sum_k Q_{ijk} = 0$$

Relations between heat loads and binary variables

$$Lb_{ij} y_{ij} \leq Q_{ij} \leq Ub_{ij} y_{ij}$$

(C2b)

Nonnegativity constraints

$$Q_{ijk} \geq 0, R_{ik} \geq 0$$
$$R_0 = R_k = 0$$

Integrality conditions for binary variables

$$y_{ij} = 0 - 1$$

Setting the binary variables to one, and defining appropriated bounds on heat load can be used to find the minimum utility cost with restricted matches combining the objective function (F1) from LP transshipment model and all the constraints from MILP transshipment model. It should be noted that in this case, the reduced model is linear since the binary variables are fixed, and it determines simultaneously the utility consumption and the heat loads of the matches, but there is no penalty in the number of units.

Cerda and Westerberg (1983) developed a MILP model based on the transportation formulation which could also handle all cases of restricted matches. The drawback of this model is that it requires more variables and constraints. Furthermore, a number of research groups suggested that in certain cases it is desirable to allow for matches between hot-to-hot and cold-to-cold process streams (Grimes et al., 1982; Viswanathan and Evans, 1987; Dolan et al., 1989), if we have cold streams at high temperature level and hot streams at low temperature level. It is worth nothing that the MILP transshipment model of Papoulias and Grossmann (1983) does not take into account such alternatives.

The minimum number of matches problems may have more than one optimal solution exhibiting the same number of matches. To establish which solution is more preferable, Gundersen and Grossmann (1990) proposed as criterion the vertical heat transfer from the hot composite curve to the cold composite curve with the key of the minimization of the total heat transfer area. The basic change is that in this model, the enthalpy interval is also partitioned into intervals. The partitioning considers all kick points of both hot and cold composite curves and draw vertical lines of these kick points. The basic idea is to compare the heat loads of vertical heat transfer, with the heat loads on the matches. If the heat loads of the matches are larger than the maximum loads of the vertical heat transfer, the objective function is augmented with a penalty term which attempts to drive the heat load of the matches down to the maximum vertical heat transfer loads defined in equation (3.4).

$$Q_{ij}^{V} = \sum_{\substack{l \in Enthalpy \\ Intervals}} \left\{Q_{il}^{H}, Q_{jl}^{C}\right\} \tag{3.4}$$

Problem P2a: MILP Transshipment for Vertical Heat Transfer (Gundersen and Grossmann, 1990).

$$min \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} y_{ij} + \varepsilon \sum_{i \in HP \cup HU} \sum_{j \in CP \cup CU} S_{ij} \tag{F2b}$$

subject to

constraints on auxiliary variables

$$S_{ij} \geq Q_{ij} - Q_{ij}^{V}$$
$$S_{ij} \geq 0$$

(C2c)

weighting factor definition

$$\varepsilon = \frac{1}{\left[\sum_{i \in HP \cup HU} Q_i\right]}$$

Constraints C2a and C2b from MILP transshipment Model

This problem was extended by Gundersen, Duvold and Hashemi-Ahmady (1996) to penalize streams with poor film heat transfer coefficient (P2b).

Problem P2b: Vertical MILP extended (Gundersen, Duvold and Hashemi-Ahmady, 1996).

$$\underbrace{min\ \alpha \sum_{i\in HP\cup HU}\sum_{j\in CP\cup CU} y_{ij}}_{\text{Minimum Number of Matches}} + \varepsilon \sum_{i\in HP\cup HU}\sum_{j\in CP\cup CU} S_{ij} + \gamma \sum_{i\in HP\cup HU}\sum_{j\in CP\cup CU} y_{ij}\left[1 - min\left(\frac{h_i}{h_j},\frac{h_j}{h_i}\right)\right] \quad \text{(F2c)}$$

All constraints of Vertical MILP Transshipment Model C2a,C2b,C2c

Solving one of the MILP models presented provides the Heat load distribution (HLD) and the key question that arises at this point is determine a HEN configuration that satisfies the minimum investment cost to the information provided by the targets of minimum utility cost and minimum number of matches applied in sequence.

3.2.3.3 Final HEN conception: Heat Transfer Area and HEN Structure

The main objective in this step consists in a representation of all desirable alternative HEN configurations (i.e., superstructure), which has the matches and the heat load specified by the MILP transshipment model. Its solution provides the network configuration with minimum investment cost determining the optimal, stream interconnections, stream flows rates and temperatures, and areas of heat exchangers units.

The superstructure proposed by Floudas et al. (1986) for each stream is depicted in Figure 3.7. Each input stream has a splitter that features of a number of outlet streams equal to the number of heat exchangers that are associated with this stream; each heat exchanger has a mixer at its inlet and a splitter at its outlet. The mixer is connected to input splitter and the splitters of the other heat exchangers. The splitter at the outlet of each heat exchanger is connected to the output mixer and the mixers of the other heat exchangers.

By assigning the heat capacity flowrate to all streams in the superstructure, and selectively setting some of them equal to zero, the incorporation of many interesting structures can be verified, including the alternatives of parallel, series, parallel-series or series-parallel, and bypass. In order to determine the minimum investment cost out of the many alternatives which are embedded in the HEN superstructure all possible connections must satisfy mass and energy balances, and feasibility constraints for heat exchanger, i.e. $EMAT\ (\Delta T_{min})$.

The objective function is the investment cost of the heat exchangers, and the optimization problem is a NLP since the energy balances for the mixers and heat exchangers have bilinear products of unknown flowrates of interconnecting streams with their unknown respective temperature. The objective function is also anon linear function of driving temperature forces expressed in $LMTD$ form.

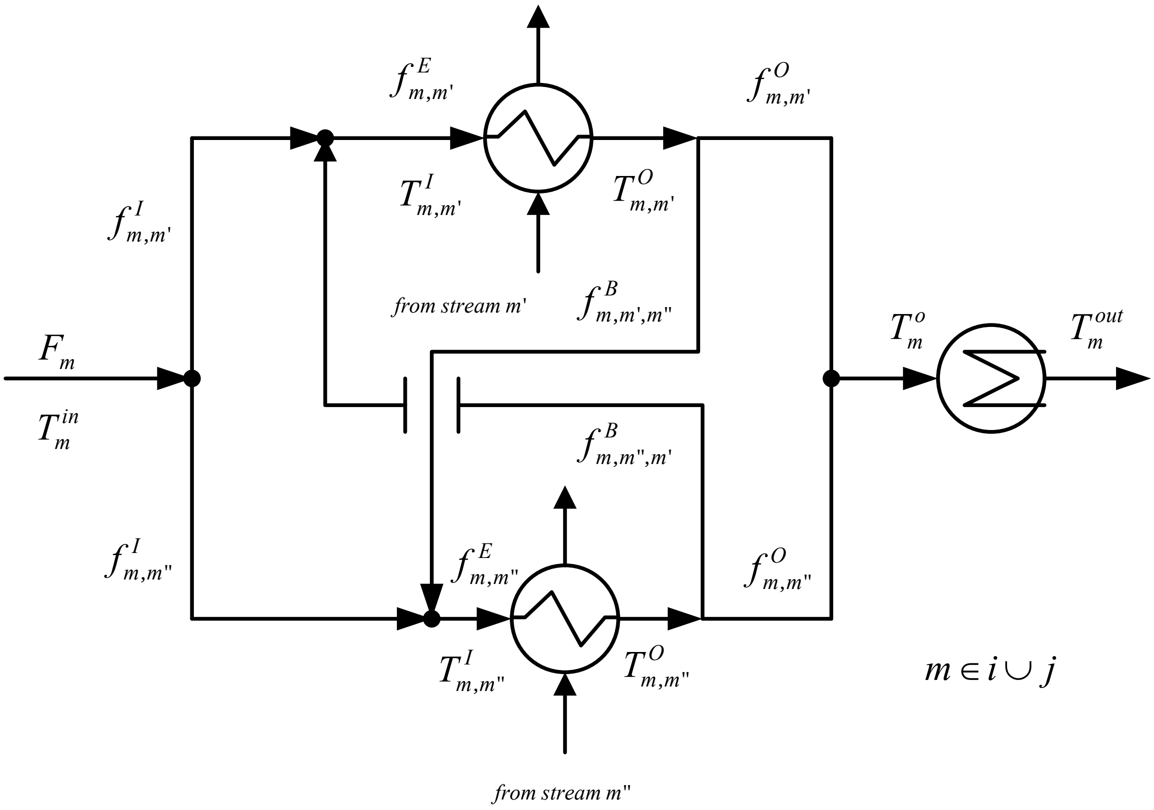

Figure 3.7: Graphical representation of the Network Superstructure.

In Floudas et al. (1986) is proofed that the minimum set of matches predicted by the MILP transshipment model corresponds to a feasible HEN solution in the proposed superstructure. Furthermore, it is showed that increasing the flows of the recycled streams tends to result in an increase of the objective function. The objective function is convex considering a given set of matches and heat loads. The heat loads can also be treated as variables since they participate linearly in the energy balances, with the penalty that the objective function no longer satisfies the property of convexity.

A very important issue for solving this model is the correct handling with the driving forces since the $LMTD$ calculation may cause numerical difficulties arising because the zero division when the driving forces at both ends of an exchanger are equal. In order to avoid such numerical difficulties, two main good approximations have been developed for the $LMTD$ calculation, the Paterson approximation (1984) presented in equation (3.5) and Chen (1987) approximation presented in equation (3.6).

Problem P3: NLP Superstructure (Floudas, Ciric, and Grossmann, 1986).

Minimum Investment Cost – Superstructure

$$\min \sum_{i\in HP\cup HU}^{nh} \sum_{j\in CP\cup CU}^{nc} c_{i,j}\left(\frac{Q_{i,j}}{U_{i,j}LMTD_{i,j}}\right)^{\beta_{i,j}} \quad \text{(F3)}$$

$subject\ to$

Mass Balance for the initial split of each stream m

$$\sum_{m'} f^{I}_{m,m'} = F_m, \qquad m \in HCT$$

Mass Balance for the mixer before heat exchanger m-m'

$$f^{I}_{m,m'} + \sum_{m''} f^{B}_{m,m',m''} - f^{E}_{m,m'} = 0, \qquad m \in HCT$$

Mass Balance for the split after heat exchange m-m'

$$f^{O}_{m,m'} + \sum_{m''} f^{B}_{m,m',m''} - f^{E}_{m,m'} = 0, \qquad m \in HCT \quad \text{(C3a)}$$

Heat Balance for mixers before heat exchange m-m'

$$f^{I}_{m,m'}T^{in}_{m} + \sum_{m''} f^{B}_{m,m',m''}T^{O}_{m,m''} - f^{E}_{m,m'}T^{I}_{m,m'} = 0, \qquad m \in HCT$$

Heat Balance for exchangers i-j hot size

$$Q_{i,j} - f^{EH}_{i,j}\left(T^{IH}_{i,j} - T^{OH}_{i,j}\right) = 0\ , i \in HP, j \in CP$$

Heat Balance for exchangers i-j cold size

$$Q_{i,j} - f^{EH}_{i,j}\left(T^{OC}_{i,j} - T^{IC}_{i,j}\right) = 0\ , i \in HP, j \in CP$$

Definitions of temperature approaches in the exchanger i-j

$$dt^{1}_{i,j} = T^{IH}_{i,j} - T^{OC}_{i,j}\ , \qquad dt^{2}_{i,j} = T^{OH}_{i,j} - T^{IC}_{i,j}, i \in HP, j \in CP$$

Minimum temperature approaches constraints

$$dt^{1}_{i,j} \geq EMAT\ , \qquad dt^{2}_{i,j} \geq EMAT, i \in HP, j \in CP \quad \text{(C3b)}$$

LMTD definition for Heat Exchangers

$$LMTD_{i,j} = \frac{dt^{1}_{i,j} - dt^{2}_{i,j}}{\ln\left(\dfrac{dt^{1}_{i,j}}{dt^{2}_{i,j}}\right)}, \qquad i \in HP, j \in CP$$

Nonnegativity constraints

$$f^{I}_{m'}, f^{E}_{m,m''}, f^{O}_{m,m''}, f^{B}_{m,m',m''} \geq 0, m \in HC\ f^{I}_{m}\ , f^{E}_{m}\ , f^{O}_{m}\ , f^{B}_{m,m'}\ \geq 0 \quad ; \quad m \in HCT \quad \text{(C3c)}$$

In the equations (3.5) and (3.6) ΔT_1 and ΔT_2 corresponds driving forces at ends of heat exchangers. The Chen approximation has the advantage that either ΔT_1 or ΔT_2 equals to zero, then the $LMTD$ is approximated to be zero, while the Paterson (1984) approximation yields a nonzero value. While the first approximation tends to slightly underestimate the area, the second one slightly overestimates it (Floudas, 1995).

$$LMTD = \frac{2}{3}(\Delta T_1 \Delta T_2)^{\frac{1}{2}} + \frac{1}{3}\left(\frac{\Delta T_1 + \Delta T_2}{2}\right) \tag{3.5}$$

$$LMTD = \left[(\Delta T_1 \Delta T_2)\left(\frac{\Delta T_1 + \Delta T_2}{2}\right)\right]^{\frac{1}{3}} \tag{3.6}$$

Solving the model $(P3)$ determines a minimum investment cost and the network configuration automatically.

3.2.3.4 Synthesis Strategy

The basic idea in the HEN synthesis strategy of Floudas et al. (1986) is to decompose the problem into the three tasks presented. The assumptions are that the energy cost is dominant, and the minimum number of units that meets the minimum energy demand is close to the minimum investment solution. The global approach presenting the steps of the synthesis along with the optimization HRAT is shown in Figure 3.8.

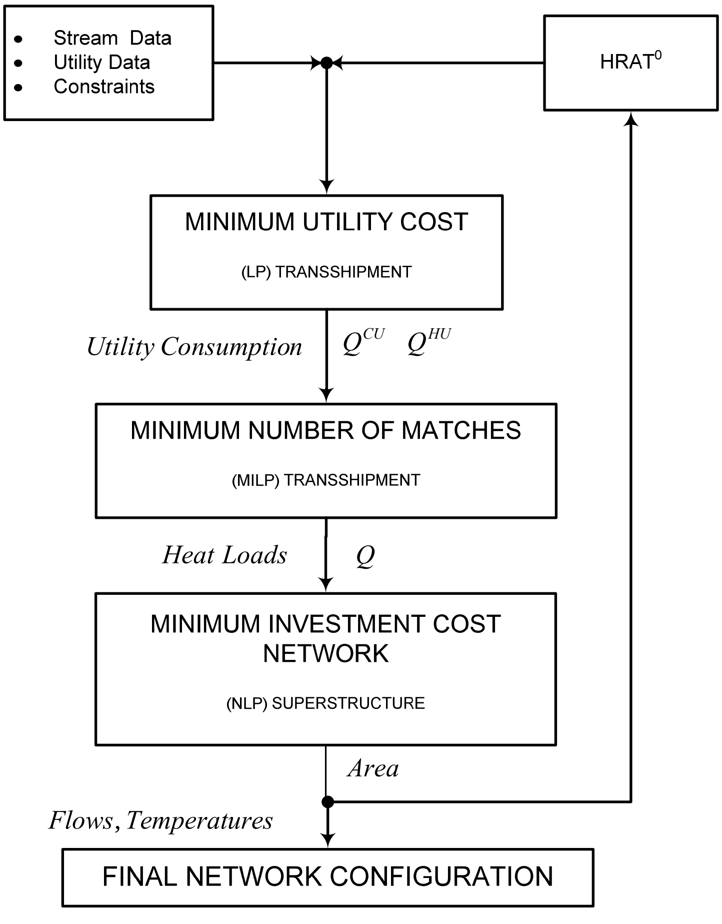

Figure 3.8: Steps of decomposition based HEN synthesis approach.

For a given initial value of $HRAT = HRAT^0$ and the problem data (i.e., stream data, utility data, and constraints) the three optimization problems are sequentially solved. The $EMAT$ can be relaxed such that $EMAT$ equals to a small positive number. At the end of this sequence, the $HRAT$ value can be updated by performing a one-dimensional search. The user can study several networks for different values of $HRAT$..

3.2.4 Simultaneous Synthesis

The decomposition described in Figure 3.8 was motivated by the analogy with the pinch technology and the inability in the 80's to address the HEN synthesis as a single task problem. But the primary limitation of sequential synthesis methods is that the different costs associated with the design of HENs cannot be optimized simultaneously, and as a result the tradeoffs are not taken into account appropriately, and sequential synthesis can often lead to suboptimal networks.

In this context, simultaneous approaches were developed in the early 90's. They involve solving HENs with little or no decomposition. These methods are primarily MINLP formulations. Floudas and Ciric (1989) proposed a simultaneous match-network synthesis problem to solve for the matches, the heat load distribution, and the network configuration all at the same time using the same superstructure illustrated in Figure 3.7. In this problem, the utility consumption is provided and the target of minimum number of matches is not used as a heuristic to determine the matches and heat loads. The representation of all possible matches and all alternative HEN configurations is denoted as hyperstructure. It has a similar topology of the superstructure, but since the matches are not known, all possible streams interconnections and heat exchangers must be represented.

In the simultaneous match-network for the strict pinch case, in which artificially do not allow for heat flow across the pinch and decompose the problem into subnetworks, the $EMAT$ is equal to $HRAT$. However, in the pseudo-pinch case, heat is allowed to flow across the pinch point if the trade-offs between investment and operating costs suggest it, $HRAT$ is greater than $EMAT$ and the problem is not decomposed into subnetworks.

Ciric and Floudas (1990) proposed an approach for the pseudo-pinch case, and through several examples demonstrated the effect of allowing heat across the pinch. An important consequence of this permission is that the optimal HEN structures obtained in that work are simple and do not feature bypass streams, resulting in more interesting structures from the practical point of view. An approach without any decomposition was proposed by Ciric and Floudas (1991). The mathematical formulation is quite similar to the match-network approach, but the utility loads are treated as unknown variables and there is no need for the optimization loop of $HRAT$ since the utility loads are determined directly.

The mathematical formulation of Ciric and Floudas (1989) is practically the same of Ciric and Floudas (1991) considering the heat utility loads (Q_i^{HU} and Q_j^{CU}) fixed as parameters defined by the LP transshipment model. As a result in the model there is no need of the heat utility load equations (constraints C4a) and in the objective function only the first term is considered resulting in the investment cost.

Problem P4: MINLP Hyperstructure Model (Circ and Floudas, 1991).

Minimum Total Annual Cost – Hyperstructure

$$\min \sum_{i \in HP \cup HU}^{nh} \sum_{j \in CP \cup CU}^{nc} c_{i,j} y_{i,j} \left(\frac{Q_{i,j}}{U_{i,j} LMTD_{i,j}} \right)^{\beta_{i,j}} + \sum_j Ccu_j Q_j^{CU} + \sum_i Chu_i Q_i^{HU} \quad \text{(F4)}$$

$subject\ to$

All Constraints from MILP transshipment Model

All Constraints from NLP Superstructure Model

Utility Loads

$$Q_i^{HU} = \sum_k Q_{ik}^{HU}, i \in HU$$

$$Q_j^{CU} = \sum_k Q_{jk}^{CU}, j \in CU \quad \text{(C4a)}$$

Feasibility Constraints for Heat Exchangers

$$f_{i,j}^{EH} - F_i y_{i,j} \le 0, f_{i,j}^{EC} - F_j y_{i,j} \le 0, i \in HP, j \in CP$$

$$f_{i,j}^{EH} \ge \frac{Q_{i,j}}{\Delta T_{i,j}^{max}}, f_{i,j}^{EC} \ge \frac{Q_{i,j}}{\Delta T_{i,j}^{max}}, i \in HP, j \in CP \quad \text{(C4b)}$$

Integrality conditions for binary variables

$$y_{i,j} = 0 - 1$$

The solution of the MINLP models provide the hot and cold utility loads, the matches and its heat loads, the areas of exchangers, the network topology with the total annual cost simultaneously.

Yee and Grossmann (1990) proposed an alternative approach for HEN synthesis without decomposition proposed by Ciric and Floudas (1991). They postulated a simplified superstructure, called SYNHEAT model, with the assumption of a stage-wise representation and isothermal mixing at the end of each stage. The main motivation behind the development was to come up with a mathematical model that features only linear constraints while the nonlinearities appear only in the objective function.

The assumption of isothermal mixing eliminates the need for energy balances in internal mixers and heat exchangers, and an energy balance per stage is used instead. These benefits are, however, accompanied by the drawback of eliminating a consideration number of HEN structures. Nevertheless, as it has been illustrated by Yee and Grossmann (1990), despite this simplification, good HEN structures can be obtained.

A simplified three stage superstructure, with two hot and two cold streams is illustrated in Figure 3.9. For each stage, each stream is split into a number of streams equal to the number of potential matches which are directed to the heat exchanger representing each potential match. The outlets flows of each heat exchanger are at the same temperature and are mixed in a point where the temperature of the considered stream at the next stage is defined. Utilities are placed at the outlets of the superstructure.

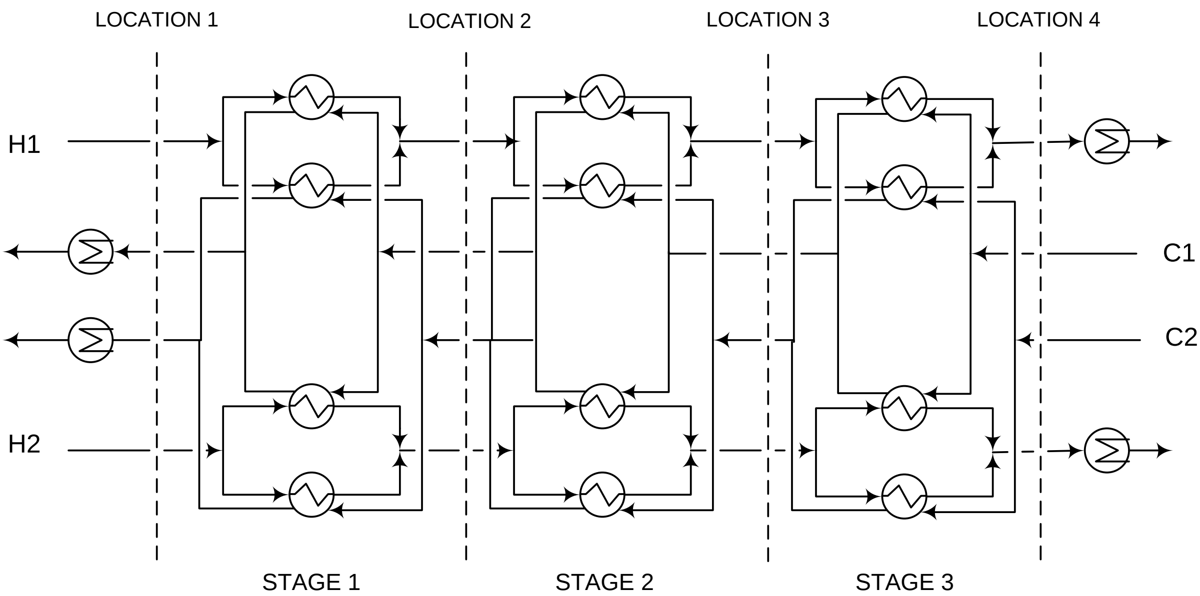

Figure 3.9: Simplified stage-wise Superstructure for HENs synthesis approach.

The outlet temperature of each stream and each stage are treated as unknown variables. Due to the isothermal mixing, those outlet temperatures are equal to the outlet temperature of each heat exchanger. The number of stages is set to equal to the maximum cardinality of the hot and cold streams. Although, as discussed by Daichendt and Grossmann (1994), sometimes it is necessary to increase the number of stages to allow designs with minimum energy consumption.

The MINLP model of Yee and Grossmann, allows nonvertical heat transfer and streams rematches, it assumes no $HRAT$, and also optimizes simultaneously capital and operating costs. The isothermal assumption reduces the mathematical representation of the feasible region to be linearly constrained. Besides the isothermal mixing, the SYNHEAT model considers: constant heat capacity flowrates, constant film heat transfer coefficients, and countercurrent heat exchangers. The $LMTD$ is originally approximated by Chen (1987) proposition. The Chen approximation, the heat transfer equation, and the concave area cost introduce nonconvexities in the model.

The global optimization of the SYNHEAT model has been addressed with a deterministic method by Quesada and Grossmann (1993) for the simplified NLP, case that assumes: fixed network configuration; linear cost; and arithmetic mean temperature difference driving forces.

Problem P5: MINLP SYNHEAT Model (Yee and Grossmann, 1990).

Minimum Total Annual Cost – Synheat Model

$$min \sum_i \sum_j \sum_k c_f z_{ijk} + \sum_i c_f z_{cui} + \sum_j c_f z_{huj} + \sum_i c_{cu} q_{cui} + \sum_j c_{hu} q_{huj} +$$

$$\sum_i \sum_j \sum_k c \left(\frac{q_{ijk}}{U_{ij} LMTD_{ijk}} \right)^{\beta} + \sum_i c \left(\frac{q_{cui}}{U_{cui} LMTD_{cui}} \right)^{\beta} \quad \text{(F5)}$$

$$+ \sum_j c \left(\frac{q_{huj}}{U_{huj} LMTD_{huj}} \right)^{\beta}$$

subject to

Overall heat balance for each stream

$$\sum_i \sum_k q_{ijk} + q_{cui} = F_i \left(T_i^{in} - T_i^{out} \right), \qquad i \in HP$$

$$\sum_j \sum_k q_{ijk} + q_{huj} = F_j \left(T_j^{out} - T_j^{in} \right), \qquad j \in CP$$

Heat balance at each stage

$$\sum_j q_{ijk} = F_i \left(t_i^k - t_i^{k+1} \right), \qquad i \in HP$$

$$\sum_i q_{ijk} = F_j \left(t_j^k - t_j^{k+1} \right), \qquad j \in CP$$

(C5a)

Assignment of superstructure inlet temperatures

$$t_i^{k=1} = T_i^{in}, \qquad t_j^{k=NOK} = T_j^{in}$$

Monotonic decrease in temperatures

$$t_i^k \geq t_i^{k+1}, \qquad t_j^k \geq t_j^{k+1}$$

$$t_i^{k=NOK+1} \geq T_i^{out}, \qquad t_j^{k=1} \geq T_j^{out}$$

Hot and cold utilities load

$$q_{cui} = F_i \left(t_i^{NOK+1} - T_i^{out} \right)$$

$$q_{huj} = F_j \left(T_j^{out} - t_j^{i} \right)$$

Minimum approach temperature constraints

$$dt_{ijk} \geq \Delta T_{min}, dt_{cui} \geq \Delta T_{min}, dt_{huj} \geq \Delta T_{min}$$

(C5b)

Logical constraints

$$q_{ijk} \geq \Omega z_{ijk}, q_{cui} \geq \Omega z_{cui}, q_{huj} \geq \Omega z_{huj}$$

$$dt_{ijk} \geq t_i^k - t_j^k + \Gamma(1 - z_{ijk})$$
$$dt_{ijk} \geq t_i^{k+1} - t_j^{k+1} + \Gamma(1 - z_{ijk})$$
$$dt_{cui} \geq t_i^{NOK} - t_{cu}^{out} + \Gamma(1 - z_{cui})$$
$$dt_{cui} \geq T_i^{out} - t_{cu}^{in} + \Gamma(1 - z_{cui})$$
$$dt_{huj} \geq t_{hu}^{out} - t_j^1 + \Gamma(1 - z_{huj})$$
$$dt_{huj} \geq t_{hu}^{in} - T_j^{out} + \Gamma(1 - z_{huj})$$

LMTD definition for Heat Exchangers

$$LMTD_{ijk} = \frac{dt_{ijk} - dt_{ijk+1}}{ln\left(\frac{dt_{ijk}}{dt_{ijk+1}}\right)}$$

$$LMTD_{cui} = \frac{dt_{ijk} - dt_{cui}}{ln\left(\frac{dt_{ijk}}{dt_{cui}}\right)}, LMTD_{huj} = \frac{dt_{ijk} - dt_{huj}}{ln\left(\frac{dt_{ijk}}{dt_{huj}}\right)}$$

Bounds

$$T_i^{out} \leq t_i^k \leq T_i^{in}, \qquad T_j^{in} \leq t_j^k \leq T_j^{out}$$
$$q_{ijk}, q_{cui}, q_{huj} \geq 0 \tag{C5c}$$

Integrality conditions

$$z_{ijk}, z_{cui}, z_{huj} = 0 - 1$$

Latter, Zamoura and Grossmann (1996) developed an approach for the MINLP case in which the fixed network configuration assumption by Quesada and Grossman is replaced by a no stream splitting assumption. This assumption can be implemented adding the inequalities (3.7) replacing the isothermal mixing assumption of Yee and Grossmann (1990) by the more stringent no stream splitting assumption.

$$\sum_j z_{ijk} \leq 1, \ \sum_i z_{ijk} \leq 1 \tag{3.7}$$

The assumption of isothermal mixing is made to avoid nonlinear constraints. A removal of the assumption introduces a number of bilinear terms. A global optimization approach with and without the isothermal mixing assumption was proposed by Bjork and Westerlund (2002). The heart of the strategy is to convexify signomial terms, and create approximate convexified subproblems. The extended SYNHEAT model includes some continuous variables, and both linear and non-convex constraints. The new variables are split ratios of the heat capacity flowrate and temperatures before mixers (Figure 3.10).

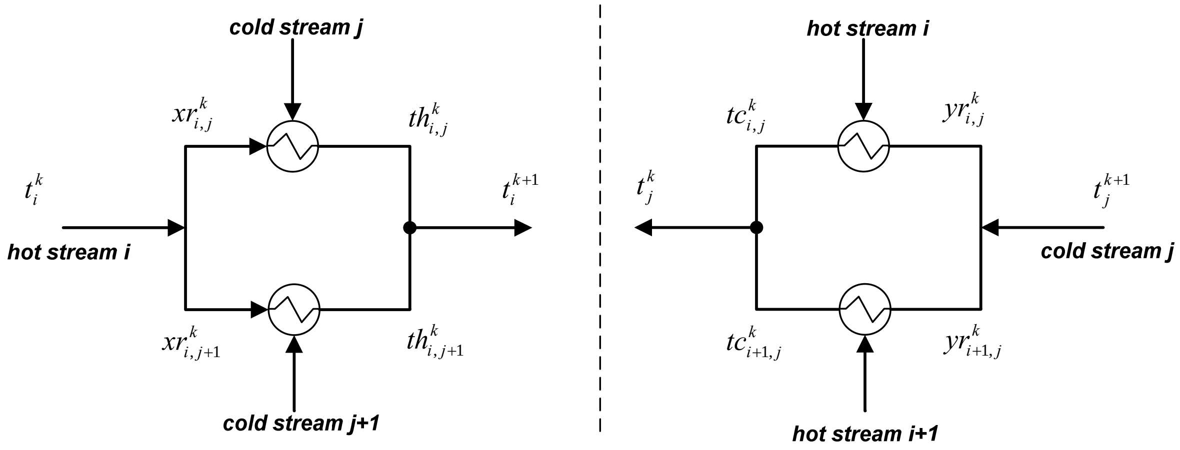

Figure 3.10: Illustration of the new variables needed for not assuming isothermal mixing.

To ensure feasible temperatures th and tc it is necessary to connect the split ratio and the temperature with the heat load. The heat balance at each stage ensures that the heat balance in the mixers is satisfied and them they are not necessary. Finally, the temperature approaches must be rewritten in terms of the new variables, and all new constraints are presented (block C5d).

Removal of isothermal mixing assumption (Bjork and Westerlund, 2002)

heat balance connecting new variables

$$q_{ijk} = xr^k_{ij} F_i \left(t^k_i - th^k_{ij} \right)$$
$$q_{ijk} = yr^k_{ij} F_j \left(tc^k_{ij} - t^{k+1}_i \right)$$

sum of split ratios

$$\sum_j xr^k_{ij} = 1, \sum_i yr^k_{ij} = 1 \qquad \text{(C5d)}$$

redefinition of temperature approaches

$$dth_{ijk} \geq t^k_i - tc^k_{ij} + \Gamma\left(1 - z_{ijk}\right)$$
$$dtc_{ijk} \geq th^k_{ij} - t^{k+1}_j + \Gamma\left(1 - z_{ijk}\right)$$
$$LMTD_{ijk} = \frac{dth_{ijk} - dtc_{ijk}}{ln\left(\frac{dth_{ijk}}{dtc_{ijk}}\right)}$$

3.3 Model Implementation and Convergence Strategy

In this work it was made an optimization overview to select the appropriated modeling system and understand how these problems can be solved (Appendix 3A). The selection of a flexible modeling system as well as the selection of suitable solvers by which a generated model can be solved is often a critical issue in obtaining valuable results in modeling applications. The choice was use the high level General Algebraic Modeling System ($GAMS$) for mathematical programming and optimization. It consists of a language compiler and a stable of integrated high-performance solvers tailored for complex, large scale modeling applications. In addition, it allows building large maintainable models that can be adapted quickly to new situations (Brooke et. al, 1998). The main HENS optimization problems described in the previous section were implemented in a systematic way using the $GAMS$ 22.2 language, the problems and the general information flow are presented in Figure 3.11.

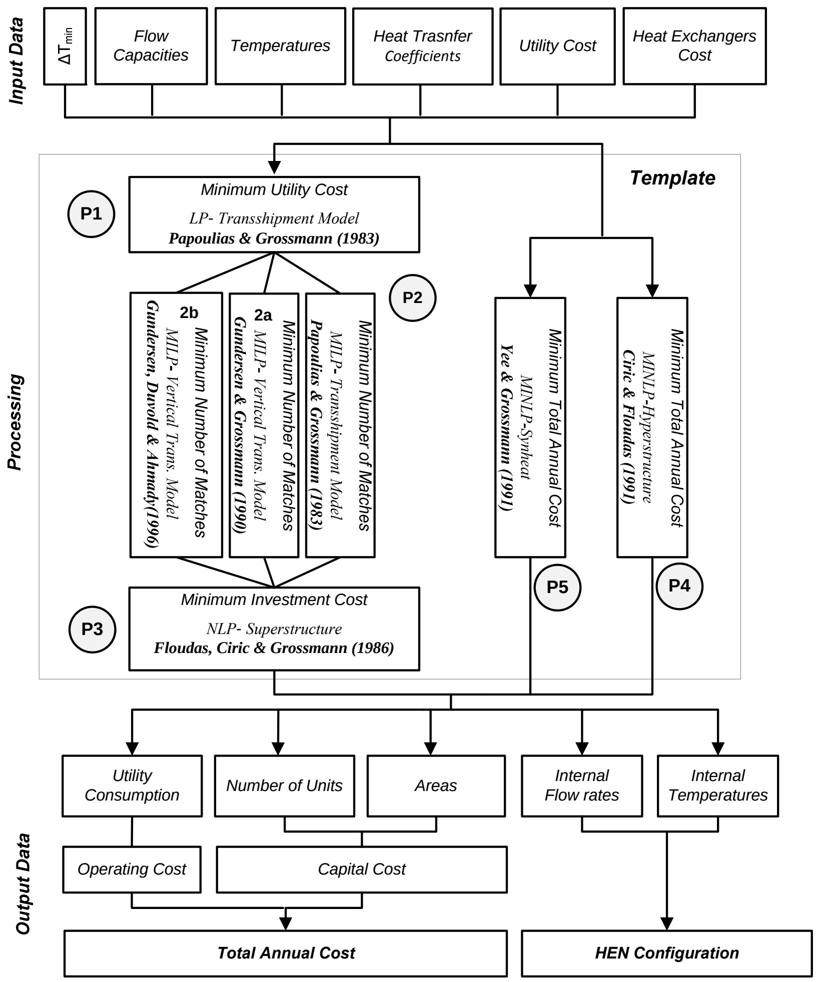

Figure 3.11: General information flow in HENS.

The systematic procedure proposed uses the same template for different input data. It implies in an automatic writing of equations based on previous information and data entry. It is important to realize that even for the LP Transshipment Model, the easier and simpler problem, the model creation depends on the data, because it defines the temperature intervals, the bounds and the necessary number of them to perform the energy balances. The same problem with different ΔT_{min} has different temperature interval bounds and possibly different number of intervals, and hence a different model structure. The MILP Transshipment Model faces the same difficulties, since it needs interval energy balances. In the NLP Superstructure case, it is necessary to create a "virtual" configuration, for which mass end energy balances are performed only when a heat load takes place, and that information is only possible when the previous step is done (MILP). The MINLP model is automatic by itself, i.e. it starts considering all possibilities contemplated by its topologies, except by the Hyperstructure that needs heat balances in temperature intervals based on external data.

3.3.1 Initialization Procedures

Solving the described optimization problems is not trivial. The LP and MILP, i.e. the linear problems, are not so complicated, since the optimization packages available can handle them even when no external initial point is given (GAMS considers zero as a default initial value if it is not defined). In the NLP case, to obtain a feasible solution is not so easy. It is necessary to bound the variables as tight as possible to decrease the feasible region. For deriving the network configuration and obtain a numerical solution of the NLP formulation it is clearly desirable to start with a "good initial guess". In the work developed by Floudas et al. (1986) an initialization procedure was proposed. This procedure might not yield an initial feasible configuration, however, it was considered in general a good initial point. The automatic synthesis procedure was implemented in the computer package MAGENETS (MAthematical Generation of heat exchanger NETwork Structures) that time, where the LP and MILP are solved with the computer code LINDO (Sharge, 1981) and the NLP was solved using the computer code MINOS (Murtagh and Saunders, 1981) by using analytical derivatives. Most common computer codes (solvers) are available in the GAMS package.

We have developed another strategy to find out the initial point that in almost cases tested guarantees the feasibility, since the previous initialization (Floudas et al., 1986) failed to solve the tested medium size problems. Initially the splits shown in the superstructure (Figure 3.7) related to flow capacities are replaced by split fractions as demonstrated in the equations in Table 3.1. Selecting feasible values (0 to 1) and substituting the definitions in the mass balance for the mixers, after some algebraic manipulation it is possible to achieve the defined linear system (mass balance in Table 3.1) to be solved to determine the heat capacity flowrate entering the heat exchangers.

After solving the mass balance for each stream it is possible to fasten all flowrates capacities defined to find the inlet temperature of the exchangers (heat balance in Table 3.1). The algebraic linear system can be found replacing the split fraction definitions in the heat balance for the mixers before the exchangers and expressing the outlet temperature in terms of the inlet temperature for each heat exchanger. The general procedure is shown in Figure 3.12. Initially, the variables are bounded as expressed in Table 3.2. The boundary step starts by the temperatures using the inlet temperatures for each process stream, and then the minimum temperature drop and the feasibility constrains involving ΔT_{min} are used to define the other bounds.

Table 3.1: Mass and Heat balance for the Superstructure using split fractions x, y.

	Mass Balance	*Heat Balance*
Hot Stream i	$f_{i,j}^{EH} - \sum_{j' \neq j} yh_{i,j',j} f_{i,j'}^{EH} = xh_{i,j} F_i$	$f_{i,j}^{EH} T_{i,j}^{IH} - \sum_{j' \neq j} yh_{i,j',j} f_{i,j'}^{EH} T_{i,j'}^{IH} = xh_{i,j} F_i T_i^{in} - \sum_{j' \neq j} yh_{i,j',j} Q_{i,j'}$
Cold Stream j	$f_{i,j}^{EC} - \sum_{i' \neq i} yc_{i',j,i} f_{i',j}^{EC} = xc_{i,j} F_j$	$f_{i,j}^{EC} T_{i,j}^{IC} - \sum_{i' \neq i} yc_{i',j,j} f_{i',j}^{EC} T_{i',j}^{IC} = xc_{i,j} F_j T_j^{in} + \sum_{i' \neq i} yc_{i',j,j} Q_{i',j}$
	Split Fraction x	*Split Fraction y*
	$xh_{i,j} = \frac{f_{i,j}^{IH}}{F_i}$ $xc_{i,j} = \frac{f_{i,j}^{IC}}{F_j}$	$yh_{i,j,j'} = \frac{f_{i,j,j'}^{BH}}{f_{i,j}^{EH}}$ $yc_{i,j,i'} = \frac{f_{i,j,i'}^{BC}}{f_{i,j}^{EC}}$

Table 3.2: Boundary values for the NLP superstructure variables.

	Temperature			*Flowrate Capacity*	
	Lower Bound	*Upper Bound*		*Lower Bound*	*Upper Bound*
$T_{i,j}^{IH}$	$T_j^{in} + \frac{Q_{i,j}}{F_j} + \Delta T_{\min}$	T_i^{in}	$f_{i,j}^{EH}$	$\frac{Q_{i,j}}{T_{i,j}^{IH,Upper} - T_{i,j}^{OH,Lower}}$	$\frac{Q_{i,j}}{T_{i,j}^{IH,Lower} - T_{i,j}^{OH,Upper}}$
$T_{i,j}^{OC}$	$T_j^{in} + \frac{Q_{i,j}}{F_j}$	$T_i^{in} - \Delta T_{\min}$			
$T_{i,j}^{OH}$	$T_j^{in} + \Delta T_{\min}$	$T_i^{in} - \frac{Q_{i,j}}{F_i}$	$f_{i,j}^{EC}$	$\frac{Q_{i,j}}{T_{i,j}^{OC,Upper} - T_{i,j}^{IC,Lower}}$	$\frac{Q_{i,j}}{T_{i,j}^{OC,Lower} - T_{i,j}^{IC,Upper}}$
$T_{i,j}^{IC}$	T_j^{in}	$T_i^{in} - \frac{Q_{i,j}}{F_i} - \Delta T_{\min}$			

The split fractions for the hot streams are initiated to maximize the temperatures of the hot side of the exchanger, i. e. setting all $yh_{i,j,j}$ to zero (maximizing the inlet temperature) and minimizing the temperature drop of all heat exchangers that involves the correspondent hot stream. That optimization problem has a analytical solution as expressed in Figure 3.12 in the block that defines the initial $xh_{i,j}$ values. By analogy, the split fractions for the cold streams are initiated to minimize the temperatures of the cold side, and hence all $yc_{i,j,i}$ are set to zero and the temperature drop is minimized.

With the initial values, the mass balance and the heat (Table 3.1) are sequentially solved for each process stream and the temperature approaches $dt_{i,j}^1$ and $dt_{i,j}^2$ are checked. If all values, for the existent heat exchangers, are positive, then a feasible solution was found and the end of the procedure is reached. Otherwise, the split fractions must be changed until it happens.

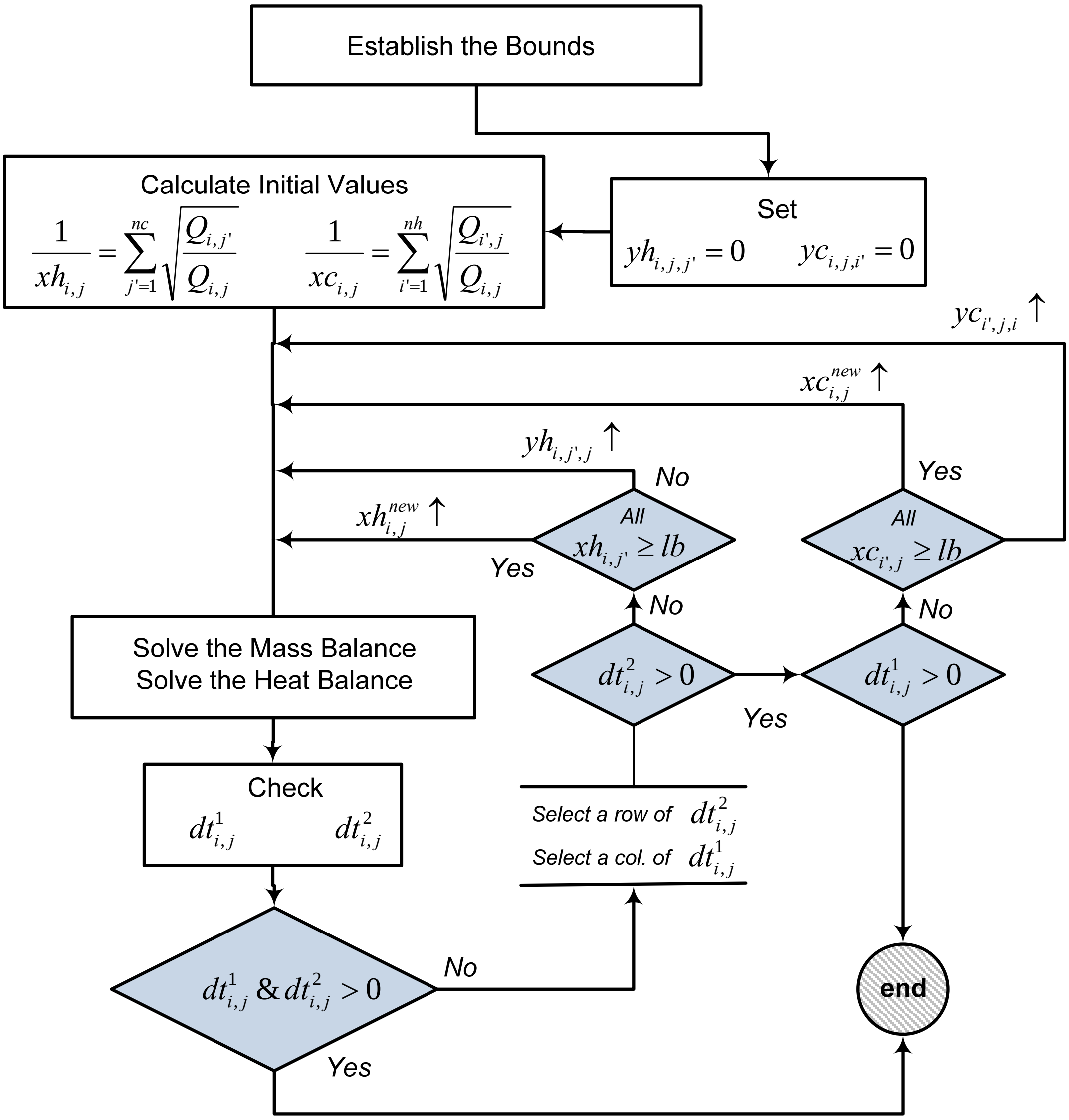

Figure 3.12: NLP initialization procedure for a feasible starting point.

Initially, it must be tried first change only the split fractions $xh_{i,j}$ and $xc_{i,j}$. It starts by the selection of the rows of $dt^2_{i,j}$ that presents negative values, and then select the most negative value in that row. Suppose the match i-j was selected, the inlet temperature of the cold stream j is already at its minimum value, but it is possible increase the $dt^2_{i,j}$value increasing the flowrate capacity entering the heat exchanger by the hot side, it implies in increasing the split fraction $xh_{i,j}$. The new value is calculated by the equation 3.8 that is easily obtained using the heat balance for the exchanger and the temperature approach definition for the current and a new situation. Using this equation the new value calculated results exactly in a temperature approach of ΔT_{min} and a small value can be used instead it to be less rigid.

$$xh_{i,j}^{new} = \frac{1}{\frac{1}{xh_{i,j}^{current}} - \frac{\Delta T_{min} - dt_{i,j}^{2}}{Q_{i,j}}} \quad (3.8)$$

To apply the new value it is necessary to check if the flowrate capacity's lower bounds for the other exchanges involving the same hot stream i are not violated, because increasing the split fraction $xh_{i,j}$ implies in decrease the split fraction $xh_{i,j'}$. If these limits are not reached the new value is applied and the procedure moves forward, otherwise we must set the maximum possible value for $xh_{i,j}$ that does not violate the bounds and increase the split fractions $yh_{i,j',j}$ from others matches, preferable the heat exchangers with the more positive values until the lower bound are achieved. The same reasoning is used to select the split fractions $xc_{i,j}$ and $yc_{i,j,i}$ and change the $dt_{i,j}^{1}$ values. Increasing the split fractions $xc_{i,j}$ promotes a bigger temperature drop and the outlet temperature of the cold stream decreases and hence increase the $dt_{i,j}^{1}$ value since the inlet temperature of the hot stream is already in its maximum value. To calculate the new values $xh_{i,j}^{new}$ an identical expression presented in equation 3.8 is used replacing $xh_{i,j}$ by $xc_{i,j}$. If the feasible solution was not found, it must be tried increase $yc_{i',j,i}$ until the lower bound is achieved.

This procedure was implemented in $MATLAB$, and it is performed in an interactive way. For any selection of the split fractions the mass and the heat balance are solved and the values for temperatures approaches are checked. Applying this procedure, it was possible to find a feasible solution for the majority of the cases tested. It must be emphasized that it increases the difficult to find feasible solutions making the feasible region tighter, but if they are not obeyed it will be not possible achieve the real areas for the exchangers.

Even when the interactive procedure fails, all the mass and heat balances are satisfied, and it is always possible at least to reduce the number of violations on the feasibility constraints. In addition, before to solve the NLP problem to minimize the capital cost, a sub problem maximizing the sum of the temperature approaches $dt_{i,j}^{1}$ and $dt_{i,j}^{2}$ subject to the mass and heat balances, is solved and the feasibility constraints using a small value of ΔT_{min} to relax the problem. The objective function is weighted using a factor proportional to the correspondent heat load, trying to maximize preferentially the temperature approaches involved in the larger heat exchangers and hence minimizing the necessary area.

The MINLPs problems involve nonlinearities and must be initialized. The aim of initialization is to prepare a problem to be successively solved in the later stages. The initialization becomes more important when the problem size increases. The general procedure is demonstrated in Figure 3.13. The Hyperstructure is solved using the Superstrucutre solution as a feasible initial point, if it was possible a previous solution, so its convergence is harnessed to NLP convergence. The Synheat Model is initialized using a sequential procedure that starts with a MILP problem adapted from the original problem ($P5$), with fixed exchangers and heat loads a NLP adapted is then solved to initialize the variables involved in the nonlinear equations and ensure the feasibility of the initial point. This systematic has been demonstrated a quite good and robust systematic approach to make possible a solution obtaining as can be seen in Section 3.5.

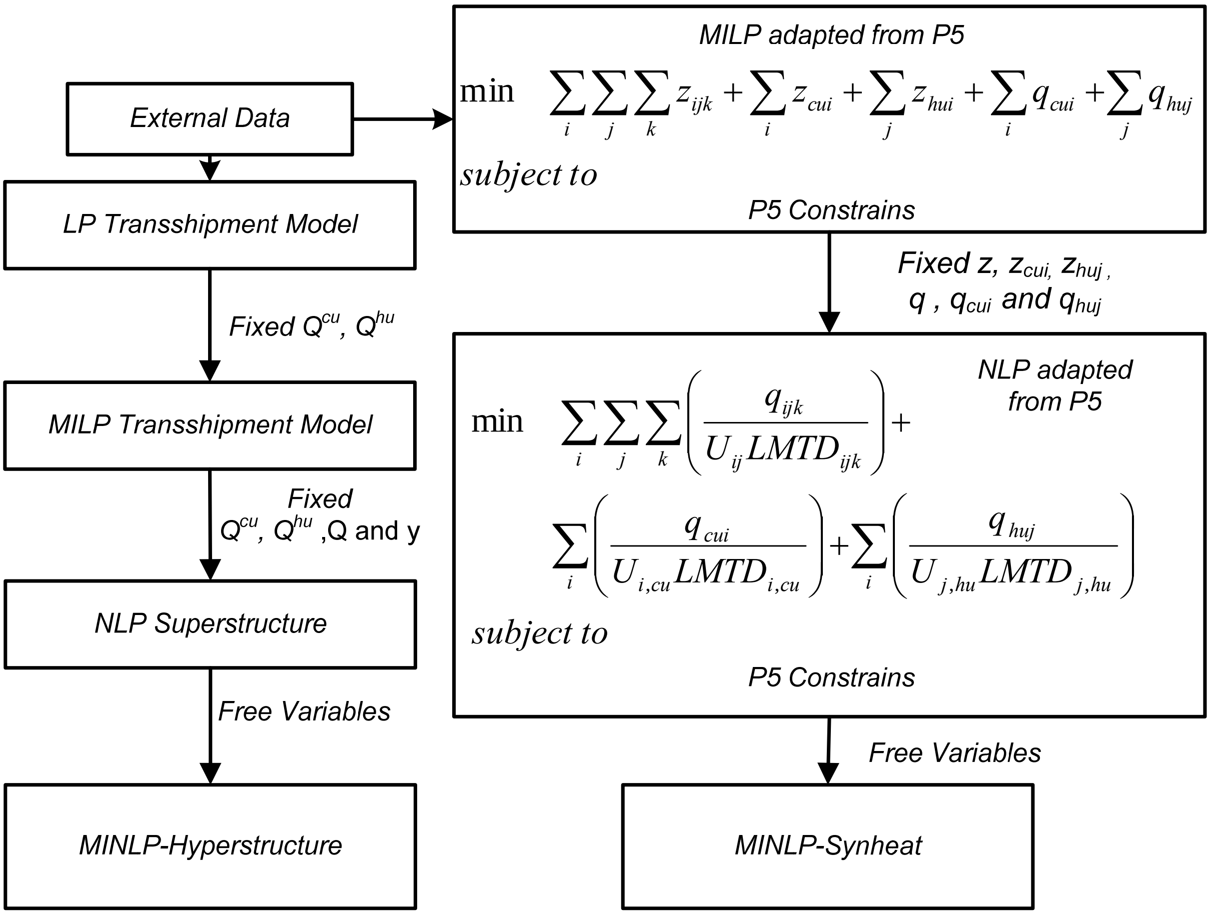

Figure 3.13: MINLPs initialization procedure for a feasible starting point.

3.4 Case Studies

Five examples from literature are presented in this section (Table 3.3 to 3.7) to illustrate the procedures and HENS models described in the previous section 3.2. The main objective is to compare qualitatively and quantitatively the whole alternatives, including numerical difficulties involved in its implementation, convergence capacity, and the quality of the final results. The problems were selected from literature with different sizes to represent beyond the complexity of the model and its behavior with different dimensions.

Table 3.3: Table 3: Problem data for Case Study 01.

Stream	T_{in} (°C)	T_{out} (°C)	F (kW°C^{-1})	h (kW m^2 °C^{-1})
H1	270	160	18	1
H2	220	60	22	1
C1	50	210	20	1
C2	160	210	50	1
CU	15	20		1
HU	250	250		1

Cost of Heat Exchangers ($y^{-1}) = 4000+500[Area (m^2)]$^{0.83}$
Cost of Cooling Utility = 20 ($kW^{-1}y^{-1})
Cost of Heating Utility = 200 ($kW^{-1}y^{-1})

Source: *Gundersern (2002)*

Table 3.4: Problem data for Case Study 02.

Stream	T_{in} (°C)	T_{out} (°C)	F (kW°C^{-1})	h (kW m^2 °C^{-1})
H1	160	93.3	8.8	1.7
H2	248.9	137.8	10.6	1.7
H3	226.7	65.6	14.8	1.7
H4	271.1	148.9	12.6	1.7
H5	198.9	65.6	17.7	1.7
C1	60	160	7.6	1.7
C2	115.6	221.7	6.1	1.7
C3	37.8	221.1	8.4	1.7
C4	82.2	176.7	17.3	1.7
C5	93.3	204.4	13.9	1.7
CU	25	40		1.7
HU	240	240		3.4

Cost of Heat Exchangers ($y^{-1}) = 4000+146[Area (m^2)]$^{0.6}$
Cost of Cooling Utility = 10 ($kW^{-1}y^{-1})
Cost of Heating Utility = 200 ($kW^{-1}y^{-1})

Source: *Chakraborty and Ghoshb (1999).*

Even the case study 05 is still not a really large problem from an industrial point of view, but it is one of the largest reported in the literature that has been addressed by mathematical programming methods.

Table 3.5: Problem data for Case Study 03.

Stream	T_{in} (°C)	T_{out} (°C)	*F* (kW°C^{-1})	*h* (kW m^{2} °C^{-1})
H1	180	75	30	2
H2	280	120	60	1
H3	180	75	30	2
H4	140	40	30	1
H5	220	120	50	1
H6	180	55	35	2
H7	200	60	30	0.4
H8	120	40	100	0.5
C1	40	230	20	1
C2	100	220	60	1
C3	40	190	35	2
C4	50	190	30	2
C5	50	250	60	2
C6	90	190	50	1
C7	160	250	60	3
CU	25	40		1
HU	325	325		2

Cost of Heat Exchangers (\$y^{-1}) = 8000+500[Area (m^{2})]$^{0.75}$
Cost of Cooling Utility / Heating Utility = 10 (\$kW^{-1}y^{-1}) / 80 (\$kW^{-1}y^{-1})

Source: *Björk and Petterson (2003).*

Table 3.6: Problem data for Case Study 04.

Stream	T_{in} (°C)	T_{out} (°C)	*F* (kW°C^{-1})	*h* (kW m^{2} °C^{-1})
H1	576	437	23.10	0.06
H2	599	399	15.22	0.06
H3	530	382	15.15	0.06
H4	449	237	14.76	0.06
H5	368	177	10.70	0.06
H6	121	114	149.60	1.00
H7	202	185	258.20	1.00
H8	185	113	8.38	1.00
H9	140	120	59.89	1.00
H10	69	66	165.79	1.00
H11	120	68	8.74	1.00
H12	67	35	7.62	1.00
H13	1034.5	576	21.30	0.06
C1	123	210	10.61	0.06
C2	20	210	6.65	1.20
C3	156	157	3291.0	2.00
C4	20	182	26.63	1.20
C5	182	318	31.19	1.20
C6	318	320	4011.83	2.00
C7	322	923.78	17.60	0.06
CU	9	17		1.0
HU	927	927		5.0

Cost of Heat Exchangers (\$y^{-1}) = 4000+500[Area (m^{2})]$^{0.83}$
Cost of Cooling Utility / Heating Utility = 25 (\$kW^{-1}y^{-1}) / 250 (\$kW^{-1}y^{-1})

Source: *Kravanja & Glavic (1997).*

Table 3.7: Problem data for Case Study 05.

Stream	T_{in} (°C)	T_{out} (°C)	F (kW°C^{-1})	h (kW m^2 °C^{-1})
H1	180	75	30	2
H2	280	120	15	2.5
H3	180	75	30	2
H4	140	45	30	2
H5	220	120	25	1.5
H6	180	55	10	2
H7	170	45	30	2
H8	180	50	30	2
H9	280	90	15	2
H10	180	60	30	2
H11	120	45	30	2
H12	220	120	25	2
H13	180	55	10	2
H14	140	45	20	2
H15	140	60	70	2
H16	220	50	15	2.5
H17	220	60	10	2.5
H18	150	70	20	2
H19	140	80	70	2
H20	220	50	35	2
H21	180	60	10	2
H22	150	45	20	2.5
C1	40	230	20	1.5
C2	120	260	35	1
C3	40	190	35	1.5
C4	50	190	30	2
C5	50	250	60	2
C6	40	150	20	2
C7	40	150	20	2
C8	120	210	35	2.5
C9	40	130	35	2.5
C10	60	120	30	2.5
C11	50	150	10	3
C12	40	130	20	1
C13	120	160	35	1
C14	40	90	35	1.75
C15	50	90	30	1.5
C16	50	150	30	2
C17	30	150	50	2
CU	25	40		2
HU	325	325		1

Cost of Heat Exchangers (\$y^{-1}) = 8000+800[Area (m^2)]$^{0.8}$
Cost of Cooling Utility = 10 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 70 (\$kW^{-1}y^{-1})

Source: *Björk and Pettersson (2003).*

3.5 Results, Analysis, and Discussion

3.5.1 Supertargeting: ΔT_{min} Selection

The first step was performing the selection of ΔT_{min} using the $Supertargeting$ procedure by Linnhoff and Hindmarsh (1983). In Figure 3.14 is presented the TAC estimated for each case study over the range of ΔT_{min} used. And the general results using Pinch Analysis to perform the targets are presented for the correspondent ΔT_{min} selected for each case are presented in Table 3.8.

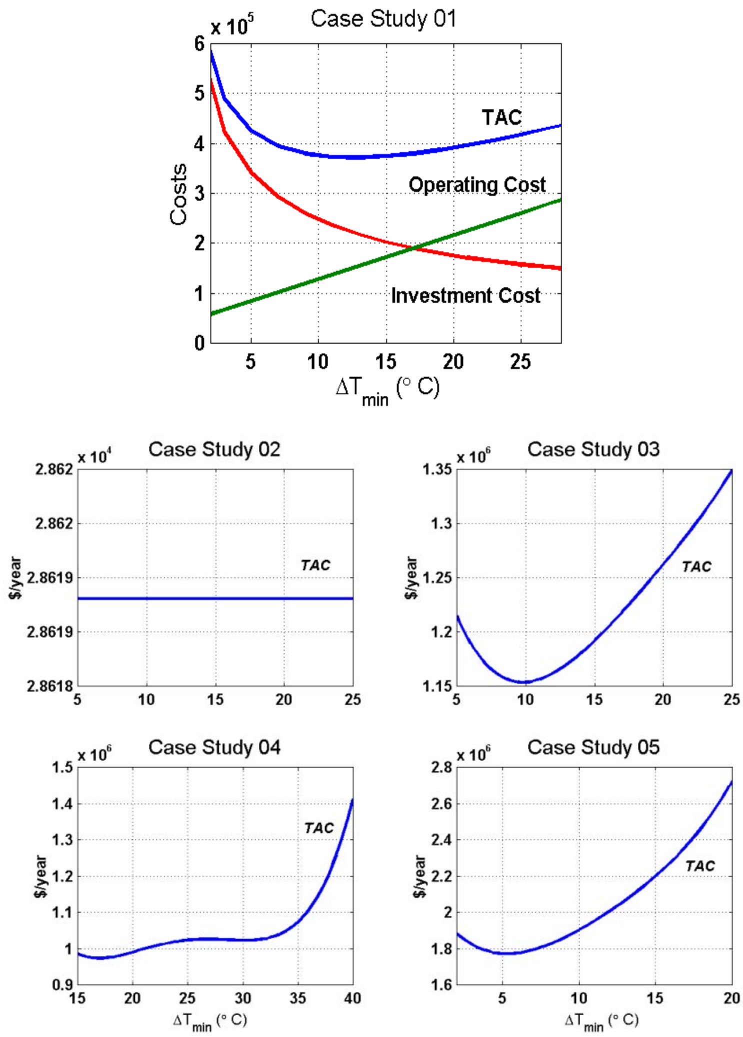

Figure 3.14: Supertargeting for all Case studies.

It could be realized that the case study 02 is not pinched for the selected ΔT_{min} since only cold utility is needed. This is due the fact that there is a threshold recognized by Linnhoff and Hindmarsh (1983), below which the problem is not pinched and either hot or cold utility usage (but not both). They called them as threshold problems. It is thus possible to apply the pinch design method to threshold problems providing the ΔT_{min} adjusted to the threshold value. Obviously the design in this case would not be too concerned about ΔT_{min} violation. However, in industrial designs, threshold problems are rare (Linnhoff and Hindmarsh, 1983).

Table 3.8: Targets obtained using the Supertargeting procedure for each case study CS.

CS	ΔT_{min} (°C)	*Pinch Temp.* (°C)	*min Hot Utility* (kW)	*min Cold Utility* (kW)	*Units* -	*Area* (m²)	*Operating Cost* ($ky⁻¹)	*Capital Cost* ($ky⁻¹)	*Total Annual Cost* ($ky⁻¹)
01	10	165	600	400	7	1226.00	128000	282732.15	470732.1
02	10	-	0	1922	10	206.0	19219.6	48967.54	68187.14
03	10	135	8900	6525	16	5280.2	747426.3	376305.37	1524678.3
04	20	130	2170	339	21	4968	550978.25	1064750.2	1615728.5
05	5	175	4450	7750	40	6782.96	1010625.00	1581442.9	1591070.1

3.5.2 Analysis of the Optimization Problems

One of the main drawbacks using mathematical programming to solve the HENS models are the explosive combinatorial nature of the problems involved. Figure 3.15 evidences that situation. For instance, the fifth case study with 39 process stream involves in its MILP transshipment model 2164 equations and 10832 variables, but even for the first case study with only 4 streams, it involves 53 equations and 69 variables for the same optimization problem.

Based on Figure 3.15 can be concluded that there are more variables than equations indicating a considerable number of degrees of freedom for the optimization. . Another point that should be noted is that not always increasing the number of streams implies that the number of variables and equations must be increased as well. In the LP the number of equations and variables depends directly on the number of temperature intervals defined automatically by the set of temperatures, when at least two temperatures are coincident, the number of temperatures interval decreases by at least one unity. For these case studies the number of temperature intervals are 8, 18, 16, 30, and 22 respectively justifying the number of variables and equations behavior for the LP case. In the MILP model exist this dependence but it is not so impacting, since in the model there are a lot of equations that depends exclusively on the number of hot and cold streams.

The NLP variables and equations does not depends at all on the number of temperature intervals, and the lower numbers, compared with the MILP model, are justified by the need of performing heat and mass balances only over the matches selected previously by the MILP model. On the other hand, in the design of the MINLP model, the equations and variables involved cannot be discarded since they virtually exist until a solution is found.

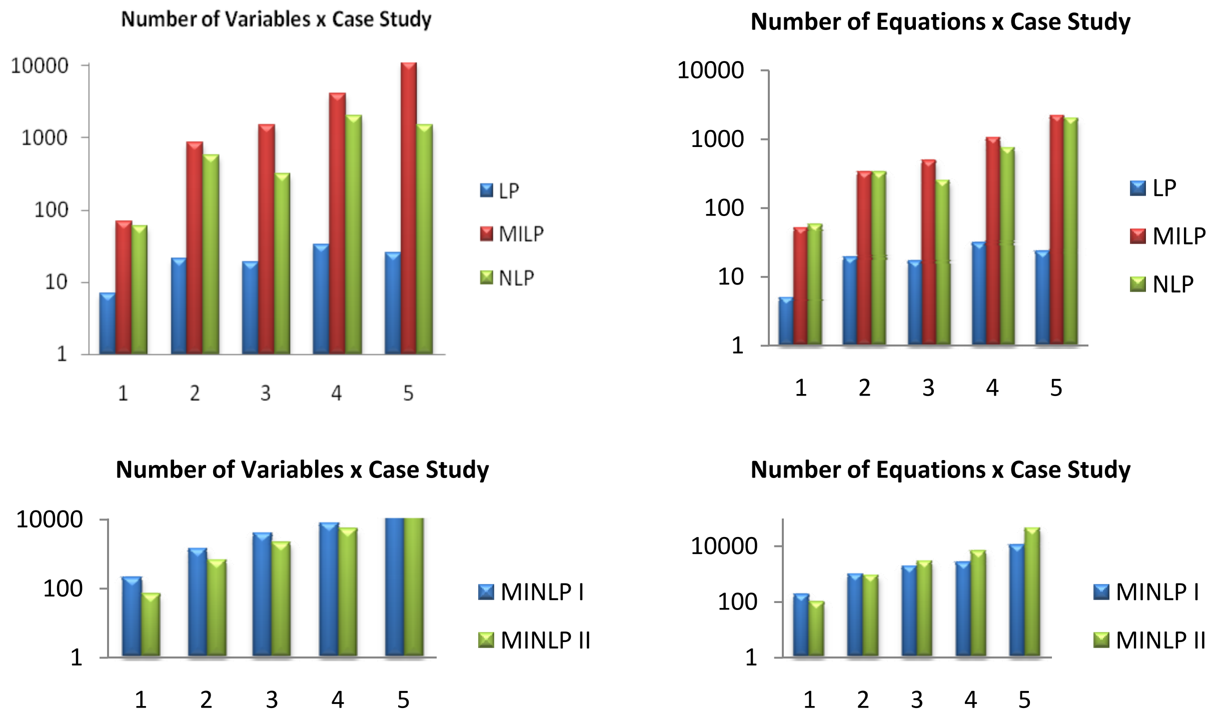

Figure 3.15: Number of variables and equations for each sequential problem (LP, MILP, NLP, MINLP I-Hyperstructure, and MINLP II-Synheat Model).

3.5.3 Solvers Selection

Solving the LP transshipment model is not a big deal and the results, i.e. the minimum utility consumption, are similar to the obtained using the supertargeting, but the main advantage of using the LP model is the possibility of considering operating constraints, and to make possible to handle forbidden and required or preferential matches.

The available licensed version of GAMS 22.2 has available 9 different LP solvers. The major solvers use the simplex method, that is a well known algorithm for solving linear programs, and the interior point methods (also referred to as barrier methods). Each solver has some particularities and different defaults and selectable options. With the case studies there were not a considerable difference among the different solvers, being all of them robust, fast and possible to find a good solution.

The selection of an appropriated solver for the MILP transshipment model using GAMS, is more delicate, since the available options have different computational efforts, time spent, and not always they converge to a solution. When it happens they are usually different, even using the same model with the same starting guesses.

With the intention of comparing different solvers – to MILP, NLP and MINLP – available to promote the best selection, in Table 3.9 is defined some indexes to perform this comparison. To all analysis was used all solvers that were available a full license, since the demo versions (free download at gams.com) restrict the maximum numbers of variables and equations disabling even the second case study to be solved. In Appendix C the most common solvers, the references and algorithm information are presented.

Table 3.9: Definitions of indexes used to compare different solvers.

$Effectiveness$	$Efficiency$	$Robustness$	$Quality$ $of\ Solution$
$\frac{100}{N}\sum_{cs=1}^{N}\frac{T_{cs}^{*}}{T_{mt,cs}}$	$\frac{100}{N}\sum_{cs=1}^{N}\frac{S_{cs}^{*}}{S_{mt,cs}}$	$100\frac{N_{mt}}{N}$	$\frac{100}{N}\sum_{cs=1}^{N}\frac{d_{cs}^{*}+\varepsilon}{d_{mt,cs}+\varepsilon}$

N is equal to the number of case studies. T refers to the computational time, S to the number of iterations, where the subscripts mt and cs refers to the method used and the case study selected. N_{mt} refers to the number of case studies solved by the method mt. The asterisk indicates the best values obtained, i.e. the lower values to T, S, and d, defined below. The parameter ε indicates the machine precision

$$d_{mt,cs} = \frac{\left\| Fobj_{mt,cs} - Fobj^{*} \right\|}{\varepsilon_{fobj}}$$

In Table 3.10 is presented the MILP solvers evaluation showing a quantitative way to select the more appropriate solver. The results indicated that the *CPLEX* is more robust, fast and obtain optimal solutions even using higher number of interaction. The weighted average considers a priority order of solving the problem (robustness – weighted with 35%) that find the optimal solution (quality – 30%) in a time-saving (effectiveness – 20%) and efficient way using little iterations (efficiency – 15 %). In addition, the efficiency was considered with the lower weight because the steps involved in each iteration for each solver are different, and therefore it is not a conclusive index in this case.

Table 3.10: MILP solver evaluation for the five case studies.

Solver	*Effectiveness (%)*	*Efficiency (%)*	*Robustness (%)*	*Quality of Solution (%)*	*Weighted Average (%)*
BDMLP	38.49	40.04	100.00	60.00	66.703
BARON	38.94	0.16	60.00	20.00	34.812
CPLEX	87.01	20.01	100.00	100.00	**85.404**
CoinGlpk	28.92	0.60	40.00	40.00	45.874
CoinCbc	5.39	80.00	80.00	80.00	65.079
weight	0.20	0.15	0.35	0.30	

The key for the methods to solve the NLP are: Successive Linear Programming (SLP), Successive Quadratic Programming (SQP), and Generalized Reduced Gradient (GRG). *CONOPT* (Drud, 1992) is a GRG method and *MINOS* (Murtagh et al., 2002) is a reduced-gradient method or a projected Lagrangian method both used to solve large scale methods. *KNITRO* is an interior point method, using SQP and trust regions. *OQNLP* and *MSNLP* are multistart heuristic algorithms that combines search methods with any NLP local solver.

BARON (Sahinidis, 1996) (Branch and Reduce Optimization Navigator) for solving non convex optimization problems to global optimality and it uses *MINOS* as NLP solver and *CPLEX* as MILP solver.

The results expressed in Table 3.11 are pointing out *MINOS* and *CONOPT* as the most robust local NLP solvers, with practically the same effectiveness and quality of solution, but in general *CONOPT* uses more iterations. The local solver *KNITRO* did not show good results. The global solvers *BARON* and *OQNLP* are robust and present satisfactory quality of solution, but they spent a lot of computational time and a high number of iterations that not even ensure the global solution. Therefore, it did not pay the computational effort.

Table 3.11: NLP solver evaluation for the five case studies.

Solver	*Effectiveness (%)*	*Efficiency (%)*	*Robustness (%)*	*Quality of Solution (%)*	*Weighted Average (%)*
BARON	36.34	80.00	80.00	40.00	59.269
CONOPT	58.44	53.21	100.00	40.00	66.670
MINOS	61.00	100.00	100.00	40.00	**74.200**
KNITRO	3.34	2.34	80.00	20.00	35.019
OQNLP	0.04	0.70	80.00	40.00	40.113
weight	0.20	0.15	0.35	0.30	

The methods to solve MINLP problem is generally based on Branch and Bound (B&B), General Benders decomposition (GBD), Outter Approximations (OA), and Logic and Disjunctives problems. *BARON* combines constraint propagation, interval analysis, and duality in its reduce arsenal with enhanced convex relaxations in a branch-and bound framework in its search for globally optimal solutions (Ryoo and Sahinidis, 1995) and (Nikolaos and Sahinidis, 2000). *DICOPT* (DIscrete and Continuous Optimizer) is based on the outer approximation method with equality relaxation strategies (Viswanathan and Grossmann, 1990). *SBB* (Bussieck and Drud, 2001) combines a standard Branch and Bound method with some of the NLP solvers in *GAMS*, e. g. *CONOPT*, *MINOS* or *SNOPT*.

Recent research has also focused on combining of Random Search (RS), such as Tabu, Scatter Search, Simulated Annealing or Genetic Algorithms, with NLP methods. *OQNLP* combines Scatter Search developed by OptTek Systems, Inc., to provide starting points for any gradient-based local NLP solver.

To evaluate the MINLP solvers were used the two models, Hyperstructure and Synheat, resulting in a double of points that were used in the MILP and NLP evaluation. The results are expressed in Table 3.12. The solver *DICOPT* presented the best performance according to the evaluation, but the *SBB* was as robust as *DICOPT* and has a similar quality of solution and efficiency, though it presented in general a slower convergence. The *BARON* and *OQNLP* did not presented good performances.

Table 3.12: MINLP solver evaluation for the five case studies.

Solver	Effectiveness (%)	Efficiency (%)	Robustness (%)	Quality of Solution (%)	Weighted Average (%)
DICOPT	79.96	53.72	90.00	70.00	**76.55**
SBB	37.10	47.10	90.00	60.00	63.99
BARON	30.36	48.24	60.00	40.00	46.31
OQNLP	11.48	35.80	60.00	10.00	31.67
weight	0.20	0.15	0.35	0.30	

3.5.4 Reporting Solutions

The best solution for each case study with each method is reported and some aspects are analyzed. To exemplify the needed decisions by solving the MILP transshipment model in Table 3.13 is illustrated three possible solutions obtained for the first case study. All solutions obtained using different solvers has the same objective function value (6 units) but they are not the same. To establish which solution is more preferable can be used the proposed criterion of vertical heat transfer, i.e. solve the modified MILP transshipment using new constraints to penalty the objective function if nonvertical heat transfer occurs.

Table 3.13: MILP transshipment model-possible solutions for the Case Study 01.

Variable	*Heat Load: Q* (kW)									
	Cold Streams									
Hot Streams	C1			C2			CU			*Total*
H1	180	0	0	1800	1800	1800	0	180	180	1980
H2	2420	2600	3200	700	700	100	400	220	220	3520
HU	600	600	0	0	0	600	-	-	-	600
Total	3200			2500			400			

**Solver order: CPLEX- CoinCbc -BDMLP all with 6 exchangers.*

In Table 3.14 is presented possible solutions using different solvers for vertical MILP transshipment model all with the same number of units foreseen by the MILP transshipment model. Table 3.15 supplies the maximum vertical heat transfer estimated from the composite curves for the Case Study 01 and the penalty term value for each solution indicating that the solution provided by *CPLEX* has the lower objective function value. It should be noted, that the maximum vertical heat transfer is a target but not a solution.

Table 3.14: Vertical MILP transshipment model-possible solutions for the Case Study 01.

Variable	*Heat Load: Q* (kW)									
	Cold Streams									
Hot Streams	C1			C2			CU			*Total*
H1	0	0	1008.57	1800	1800	971.43	180	180	0	1980
H2	3200	2600	2191.43	100	700	928.57	220	220	400	3520
HU	0	600	0	600	0	600	-	-	-	600
Total	3200			2500			400			

**Solver order BDMLP- BARON -CPLEX all with 6 exchangers.*

Table 3.15: Maximum Vertical Heat Transfer and solution for Case Study 01.

	Maximum Vertical Heat Transfer			Solution		
	C1	C2	CU	Solver	Fobj.	$\sum\sum S_{ij}$
H1	1008.57	1542.86	0	BDMLP	6.1995	0.200
H2	2591.43	1100	400	BARON	6.1433	0.143
HU	171.43	428.57	-	CPLEX	**6.0281**	**0.028**

All case studies do not show much difference in the heat film coefficient. Hence the extended MILP problem to penalize streams with poor heat coefficients does not promote big changes in the matches selected. For the first case study the solution is exactly the same using the vertical MILP. The best MILP solutions found are also presented in the Appendix 2B.

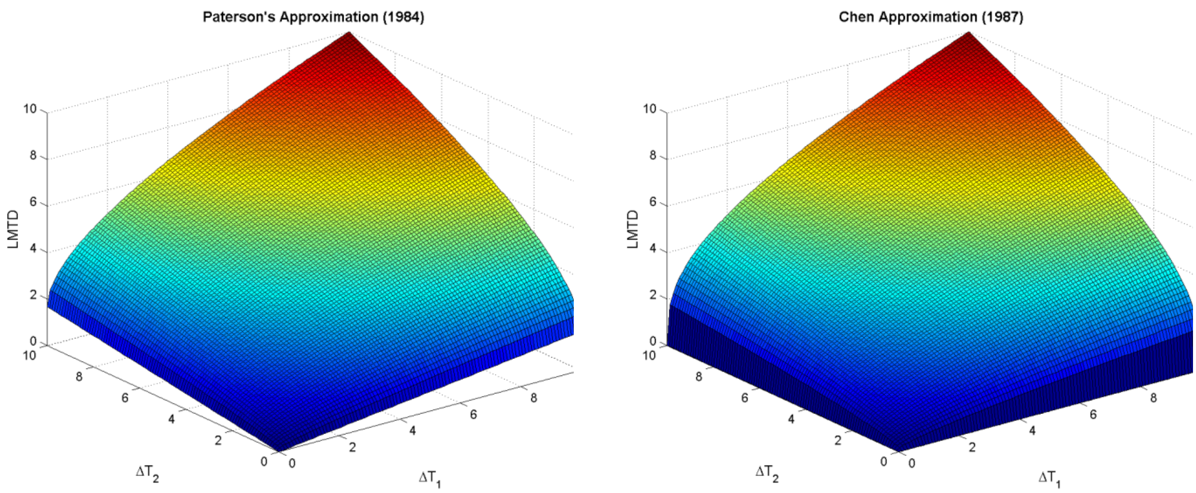

Figure 3.16: Log mean temperature approach approximations.

The two approximations to the LMTD are exhibited in Figure 3.16, where can be concluded that they are very similar but with a different behavior when at least one temperature difference tends to zero.

The general results are shown in Table 3.16 and the HEN configurations exhibited in Appendix 3A. It was possible obtain a feasible solution to all case studies using the convergence strategy demonstrated in section 3.3.

Table 3.16: General Reporting best solutions.

Case study	*Hot Utility* (kW)	*Cold Utility* (kW)	*Units* -	*Area* (m^2)	*Operating Cost*.10^{-5} ($\$ky^{-1}$)	*Capital Cost*.10^{-6} ($\$ky^{-1}$)	*Total Annual Cost*.10^{-6} ($\$ky^{-1}$)
Sequential Procedure							
01	600	400	6	1151	1.280000	0.2483872	0.3763872
02	0	1922	9	277.9	0.192196	0.0455483	0.0647679
03	8900	6525	18	6418.8	7.772500	0.8360500	1.6133000
04	2170	339	21	5430.9	5.509782	0.9672089	1.5181872
05	4450	7750	42	9627.2	3.890000	2.6972479	3.0862479
Simultaneous-Hyperstructure							
01	600	400	6	1112.2	1.280000	0.2339828	0.36198278
02	0	1922	9	273.3	0.192196	0.0455446	0.06476419
03	9304.5	6929.5	18	5618.1	0.813651	0.7612971	1.57494821
04	2170	339	21	5430.9	5.509782	0.9672089	1.51818720
05	8561	11861	43	3615.5	7.178553	1.4797979	2.19765329
Simultaneous-Synheat							
01	600	400	6	1061.8	1.280000	0.2380067	0.36600668
02	0	1922	9	254.5	0.192196	0.0451432	0.06436279
03	9924	7549	17	4513.4	8.6937454	0.6372929	1.50666740
04	1938	107	21	4895.8	4.8717270	0.9738335	1.46100620
05	6226	9526	44	3991.8	5.3107272	1.5243484	2.05542113

In addition, the simultaneous procedures always presented an improved solution comparing with the sequential procedure, except in the case study 02, where it was not possible a better solution starting with the sequential solution as initial guess. Another point is that the simultaneous solution using the Synheat model was, except by the case study 01, the best solution. It was not expected since the Synheat model restricts the search space using the isothermal mixing assumption; on the other hand, the model is linear constrained making easier to obtain a solution.

To the case study 01 was designed a HEN using Pinch Technology and the Pinch solution was used as initial point to the NLP Superstructure. The resulting HENs can be seen in Figure A.1 evidencing that was possible to improve the solution but all the optimization problems presented a better solution as can be seen in Figure A.2.

Due to the nonautomatic procedure to design the HEN using Pinch Technology, it was not tested use the solution as initial point to the other case studies. The proposed initialization strategy was applied to all cases, and the HENs configurations using the optimization techniques are presented in Appendix 3A.

3.5.5 Methods Evaluation

It was performed a qualitative/ quantitative evaluation over the optimization methods to solve the HENS problems. The results are summarized in Table 3.17. All methods are appropriated to treat the design, but they have different strong points, e.g. the Superstructure (Sequential) is easier to implement and solve and it has a lower computational effort but the solution can be improved using a simultaneous procedure.

Comparing the different simultaneous approaches, the Synheat model presented in general better indexes, being the simpler, more robust and with best solutions representing the best tradeoff. It does not mean that the simultaneous approach based on Hyperstructure should be discarded, since it shows better solutions than the sequential procedure. To complete the analysis it would be interesting check and compare some practical aspects such as operability, controllability and flexibility. It should be noted that the simultaneous approaches with no additional constraint result in general in a more complex configuration, i.e. more stream splits and recycles, which possibly difficult the operation and control.

Table 3.17: Optimization Methods for HENS Evaluation.

Solver	*Implementation Easiness* (%)	*Easiness Solution Obtaining* (%)	*Computational Effort* (%)	*Robustness* (%)	*Quality of Solution* (%)	*Average* (%)
Superstruct.	75.00	80.00	80.00	92.00	81.30	82.30
Hyperstruc.	70.00	65.00	70.00	70.00	87.20	73.40
Synheat	70.00	70.00	76.00	90.00	89.80	80.70
weight	0.20	0.15	0.35		0.30	

3.5.6 Final Remarks

During the implementation and the obtaining solution process behind the methods it was faced some difficulties that were overcome and some remarks are registered:

- The LP and the MILP need heat balances in temperature intervals. To increase the search space and hence the flexibility to find the heat loads and matches solving the MILP, it is possible use a lower HRAT even a zero value;

- Solving the MILP it is possible and interesting limit the maximum number of heat exchangers by process stream, avoiding complicated structures and decreasing significatively the number of variables in the NLP step;

- Using GAMS it is interesting to use the model property called "*holdfixed*" to fix the variables already known and pass to the solver as parameters reducing the dimension problem facilitating the problem solvability;

- Solving the NLP it is possible to provide a ΔT_{min} relaxation, even use it as a variable with a small number as its lower bound to give more flexibility to the solver allowing heat cross trough the pinch if the total annual cost suggests it;

- Solving the MINLP Hyperstructure model does not contemplate streams that not participate in the heat integration, but solving the case studies it was realized that it is much common. To overcome this problem it was created a global bypass stream that appears only in the initial split and final mixer balances;

- Solving the MINLP Synheat, *a priori* does not take into account pinch information, but it is appropriated find a solution with a utility consumption near to the foreseen by pinch analysis (or LP transshipment model), so it is interesting insert new constrains limiting the maximum consumption or use slack variables to allow more flexibility to decrease the total annual cost.

3.6 Conclusions

Although HENS has been one of the most studied problems in process synthesis, even to small problems finding feasible solution using optimization methods has been troublesome. In this present work, the main optimization methods for HENS were presented, i.e. sequential and simultaneous, and implemented using the software $GAMS$. The implementation supplies the designer with a suitable environment to solve the problems quickly, i.e. without much external intervention at the implementation step, in an easy fashion way.

A new convergence strategy for the initialization for the synthesis of HEN has been developed. This approach has been applied successfully to find out an initial feasible solution providing to the solver a good point to start the algorithm. Five case studies with different dimensions, i.e. number of process streams, were used to illustrate the implementation of the optimization methods, and the convergence strategies.

It was analyzed the appropriated solver to each particular problem using a $GAMS$ license through a quantitative comparison among the different optimization methods for HENS. For comparison purpose some indexes were used to distinguish the performances. They were based on numerical aspects, solvable capacity and quality of solution obtained. Extensive tests were performed, i.e. taking account all possible combinations (case study-solver), when a full solver license was available, resulting in 25 LPs, 25 MILPs, 25 NLP s and 40MINLPs in a total of 115 problems to be solved. The main conclusions were the $CPLEX$ solver as the best solver to linear problems, and for NLP problems the best choice has been $MINOS$ and $CONOPT$ had the best performance solving the NLP problems, very fast and robust. To solve the MINLPs the solvers $DICOPT$ and SBB was the more suitable with the best performances.

The comparison among the approaches; i.e. Superstruture, Hyperstruture and Synheat Model, was based also on indexes. Subjective indexes, such as implementation easiness and easiness solution obtaining, and based on data, such as computational effort, robustness and quality of solution. All the problems solved were used to provide a general analysis. The main conclusions are that the sequential problem is easier to solve and implement, quite robust, with a low computational effort compared with the simultaneous methods, but with a poor quality of solution since it was always possible to improve the solution using the simultaneous framework. The simultaneous methods, as it was supposed, are harder to treat, even though they present better solutions. Comparing the two different simultaneous approaches, the Synheat model presented in general a best performance, despite the isothermal mixing assumption that limits the topologies contemplated. It is due the fact that this problem is easier to solve since it is linear constrained unlike the other one.

Finally, despite the difficult involved in obtain a solution using optimization methods for HENS, the proposed systematic framework strategy was shown to find feasible and applicable solutions to all case studies for each optimization method (a total of 15 problems). Since the nonlinear problems are non-convex, only local optimum were obtained in this work but the main objective was just select an appropriated method to sequential developments, i.e. make an attempt to address beyond the costs, the operability and controllability aspects during the design step, proposing a formulation that will worth to make some effort trying to find the optimal solution and complete the analysis in a more properly scenario with an outstanding feature of taking account not only the operating and capital costs but its implementation in practical situation.

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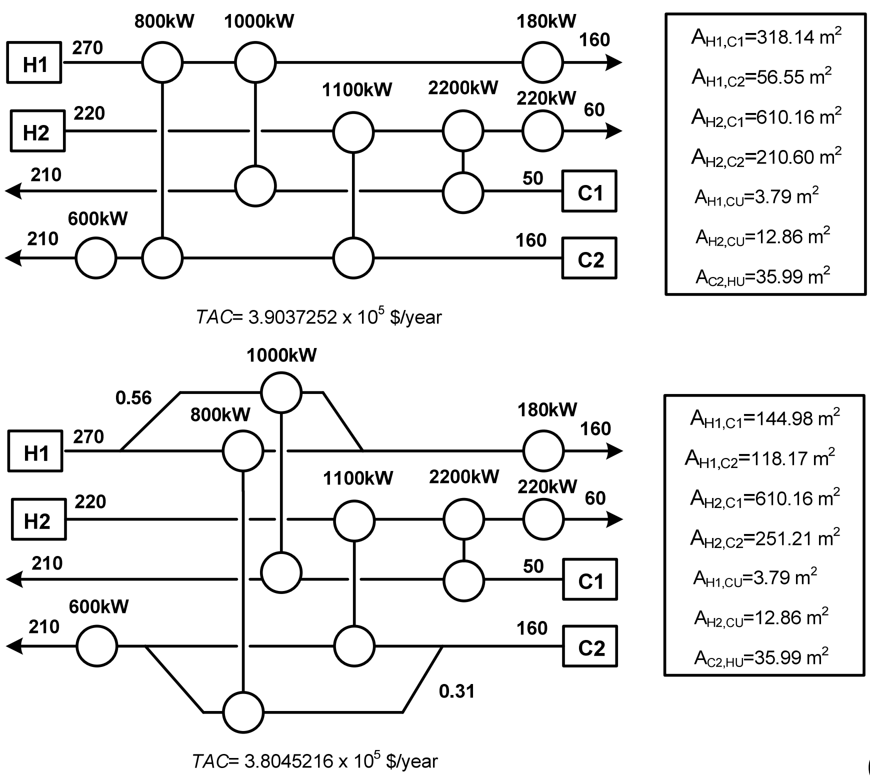
Appendix 3A

Reporting Best Solutions



(a)

(b)

Figure 3A.1: HEN configuration for Case Study 01 using Pinch Technology (a), using NLP Superstructure using Pinch Solution as initial point (b).

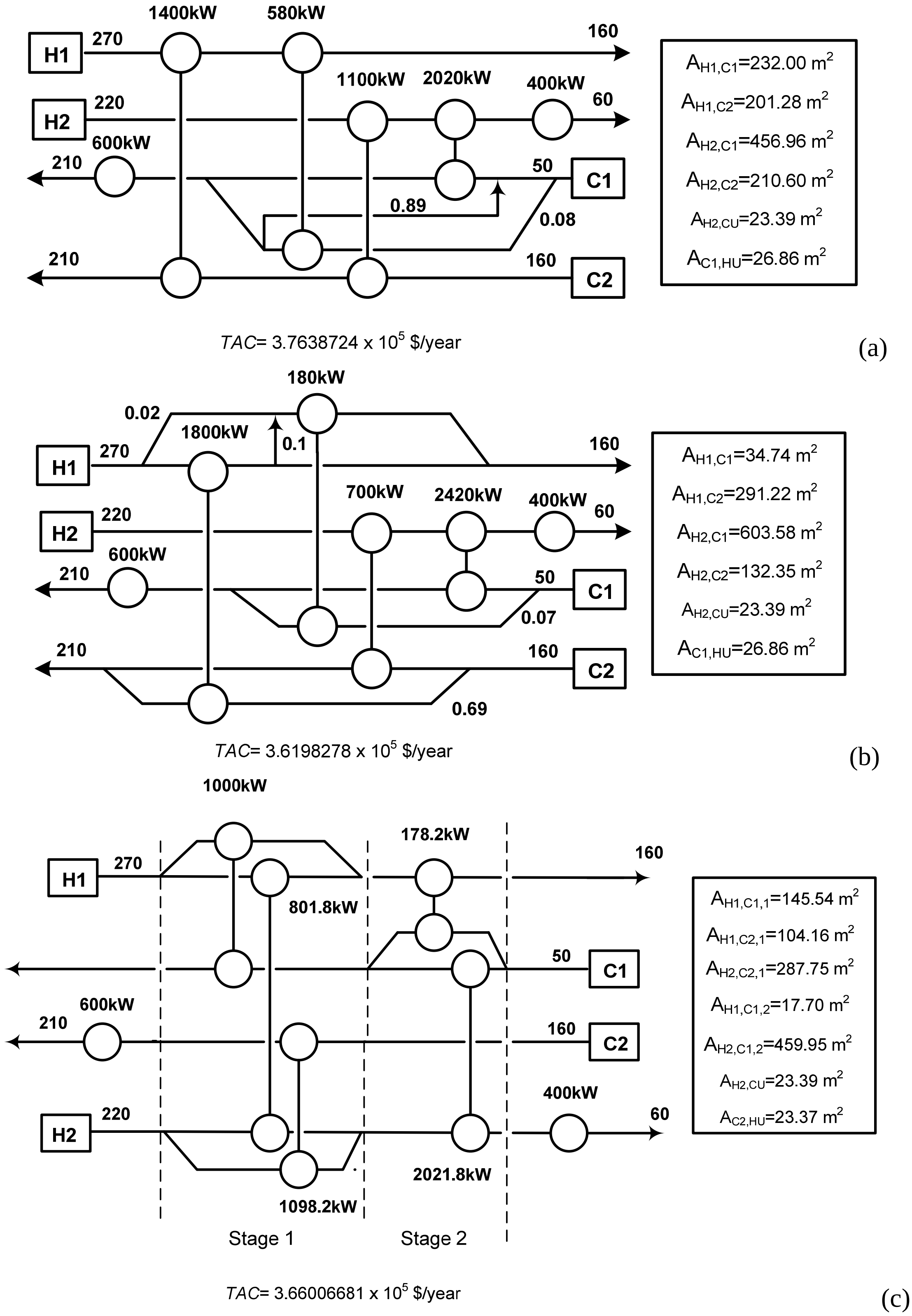


Figure 3A.2: HEN configuration for Case Study 01 using Superstructure (a), Hyperstructure (b) and Synheat Model (c).

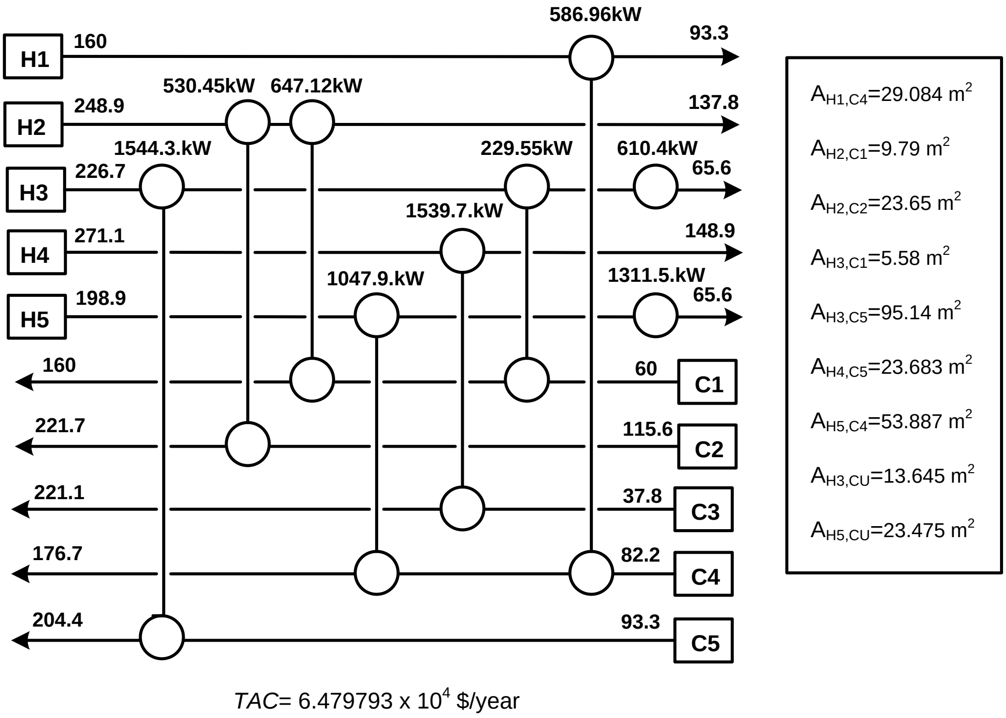


Figure 3A.3: HEN Configuration for the Case Study 02 using Superstructure.

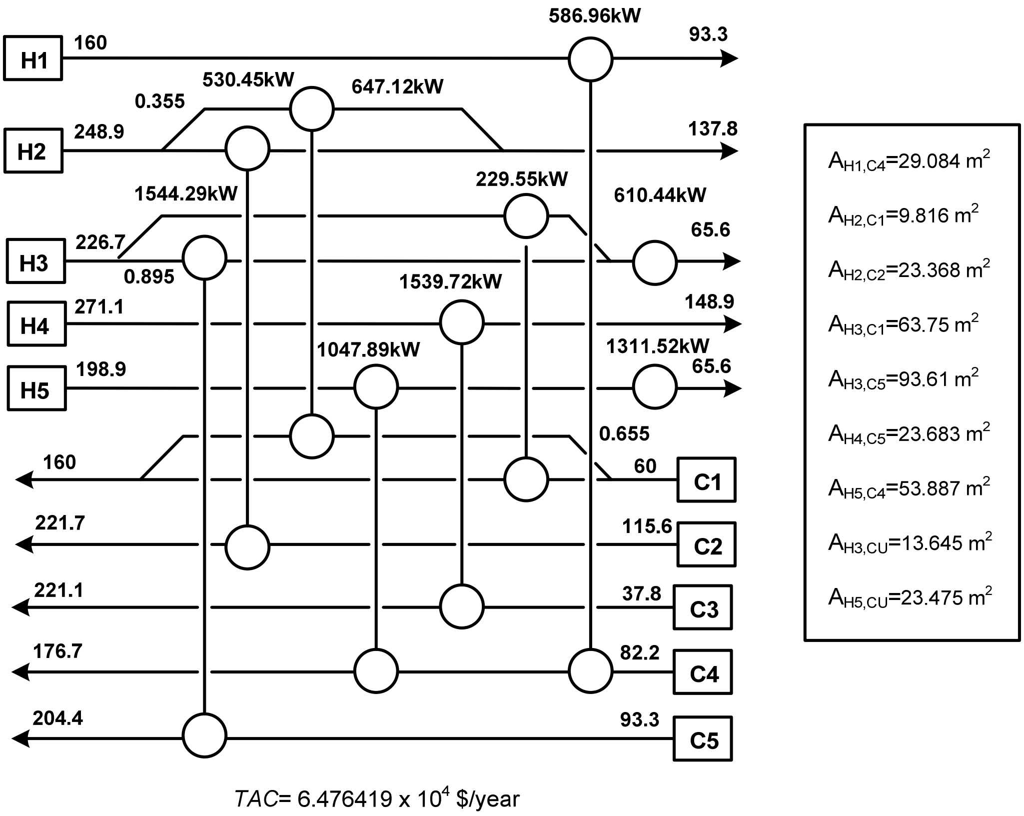


Figure 3A.4: HEN Configuration for the Case Study 02 using Hyperstructure.

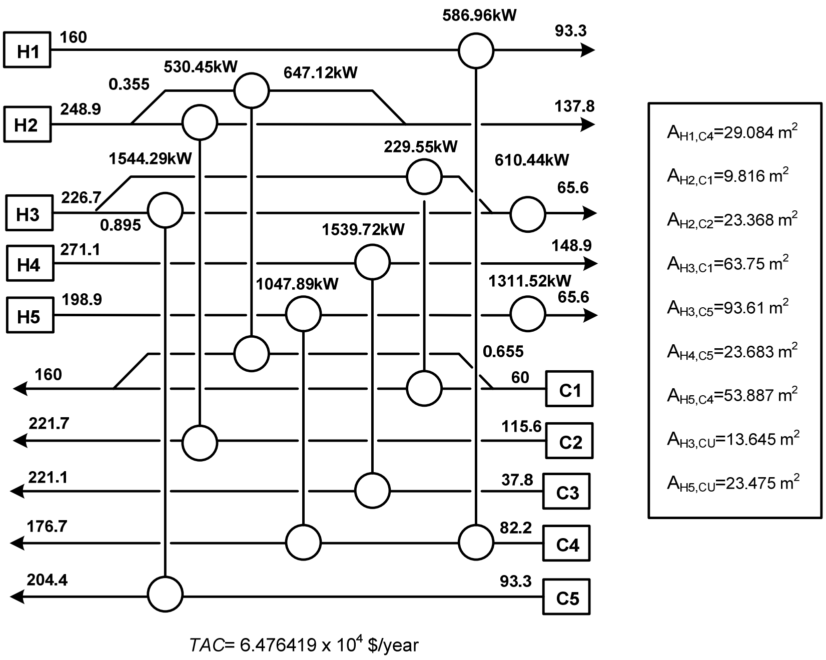


Figure 3A.5: HEN Configuration for the Case Study 02 using Synheat.

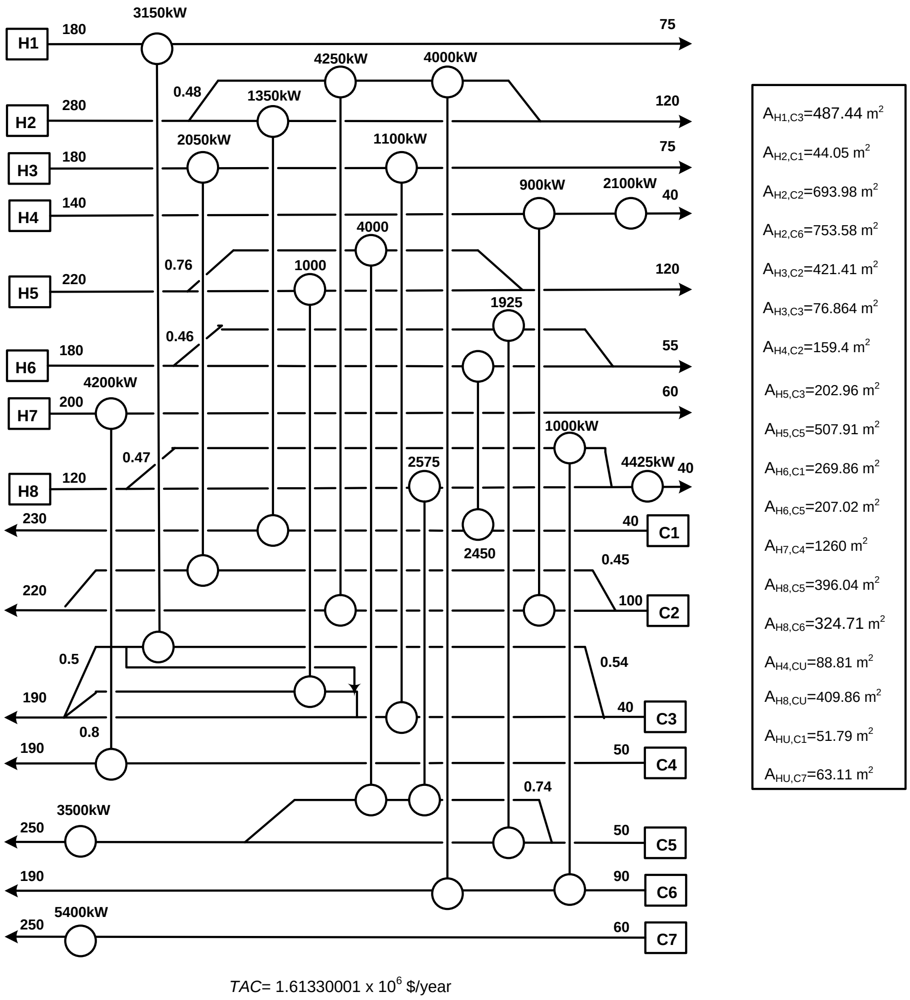
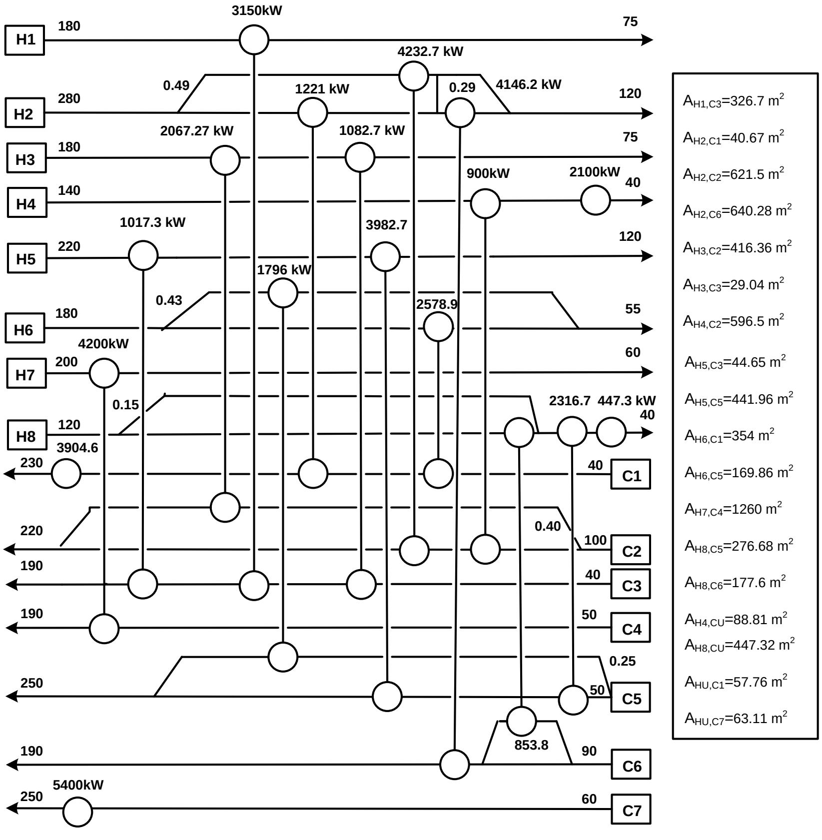
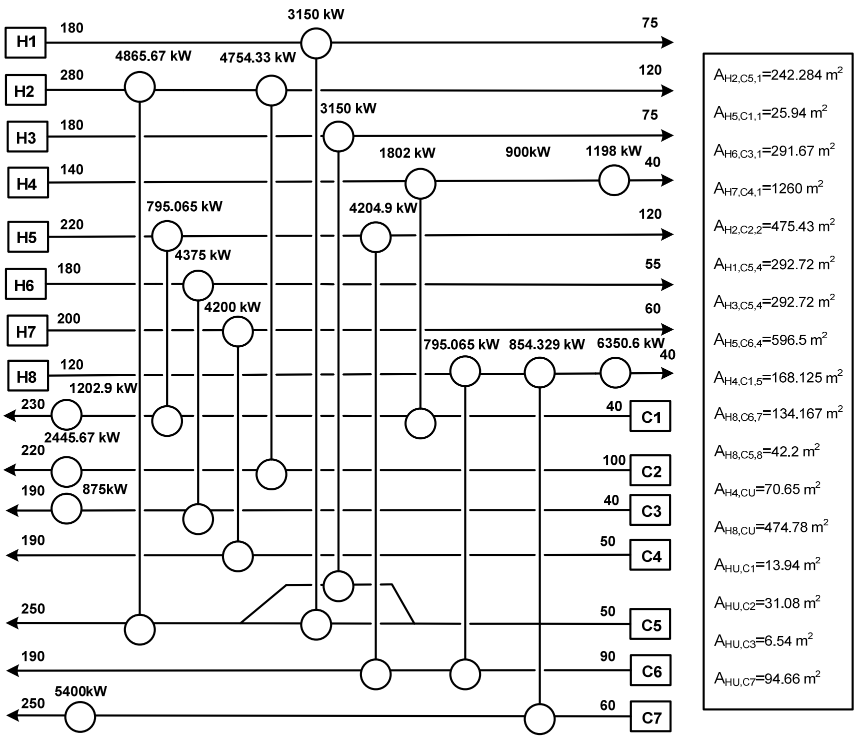


Figure 3A.6: HEN Configuration for the Case Study 03 using Superstructure.



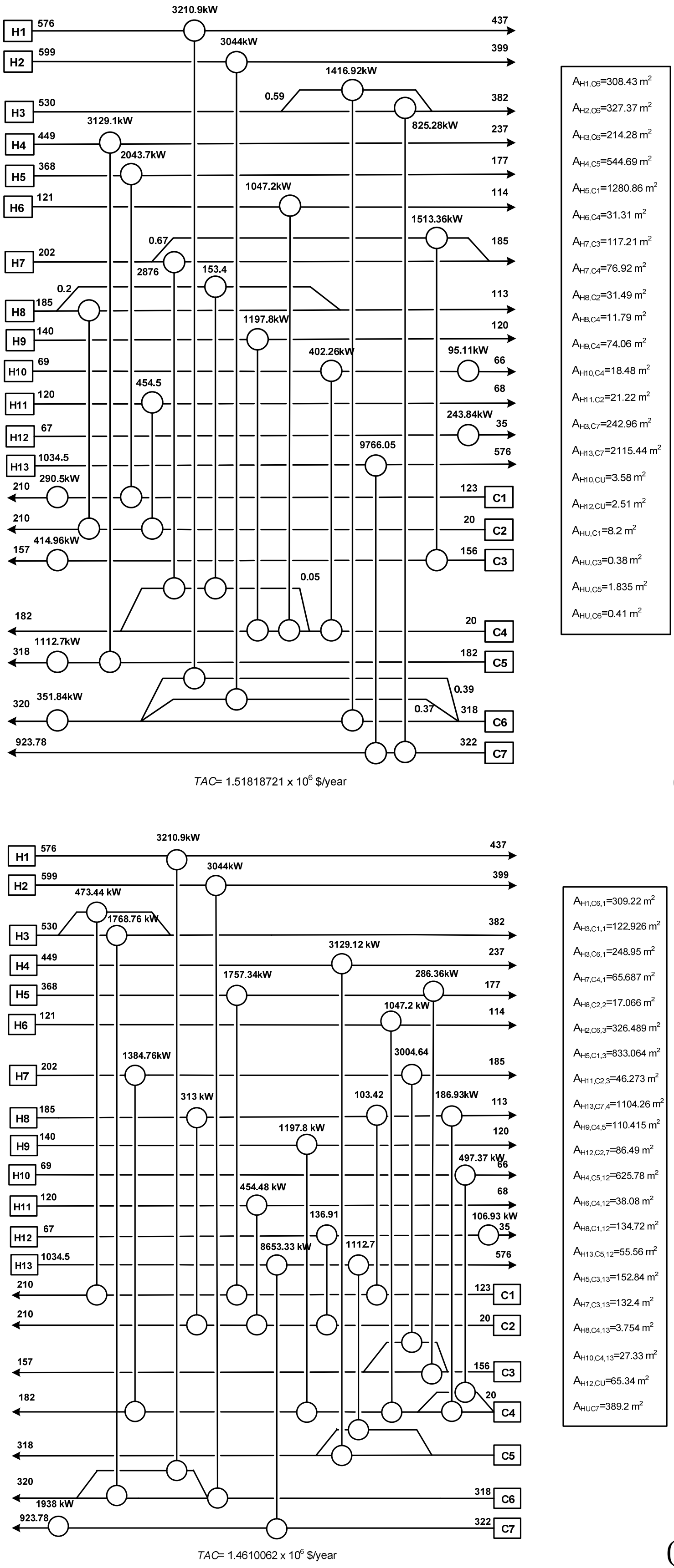
TAC= 1.57494821 x 10^6 \$/year

Figure 3A.7: HEN Configuration for the Case Study 03 using Hyperstructure.



TAC= 1.50666740 x 10^6 \$/year

Figure 3A.8: HEN Configuration for the Case Study 03 using Synheat.



(a)

(b)

Figure 3A.9: HEN Configuration for the Case Study 04 using Superstructure and Hyperstructure (a), and Synheat (b).

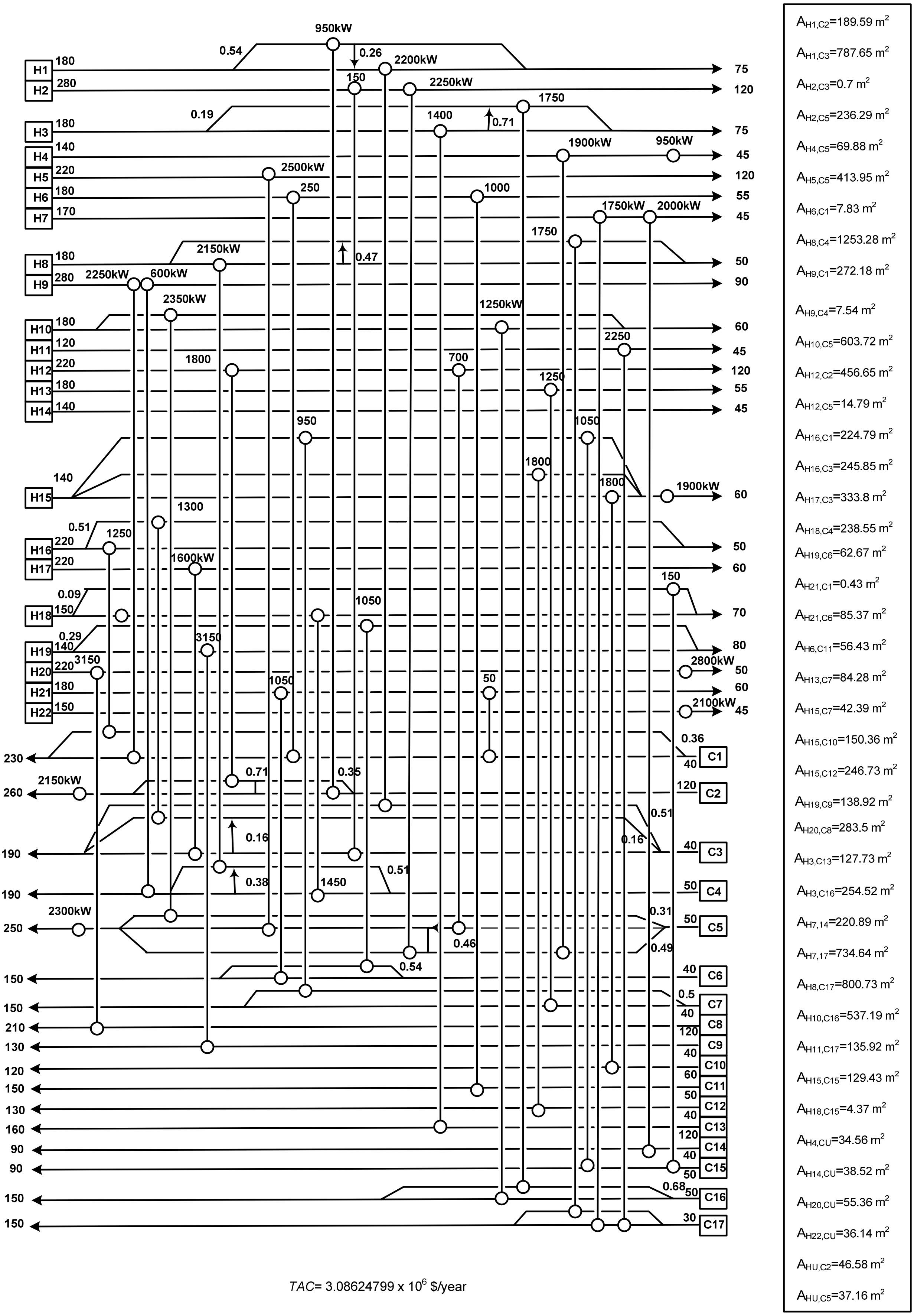


Figure 3A.10: HEN Configuration for the Case Study 05 using Superstructure.

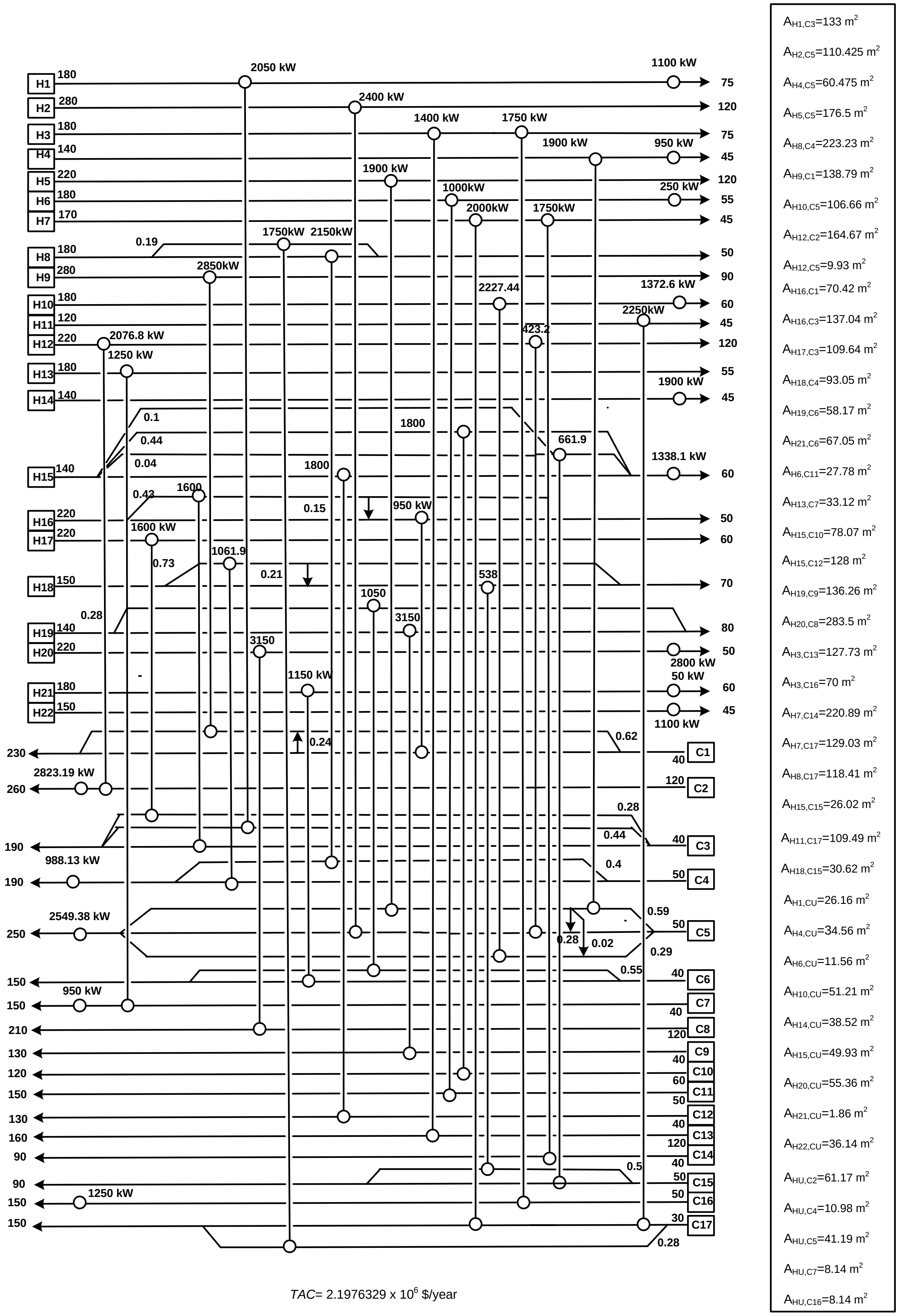


Figure 3A.11: HEN Configuration for the Case Study 05 using Hyperstructure.

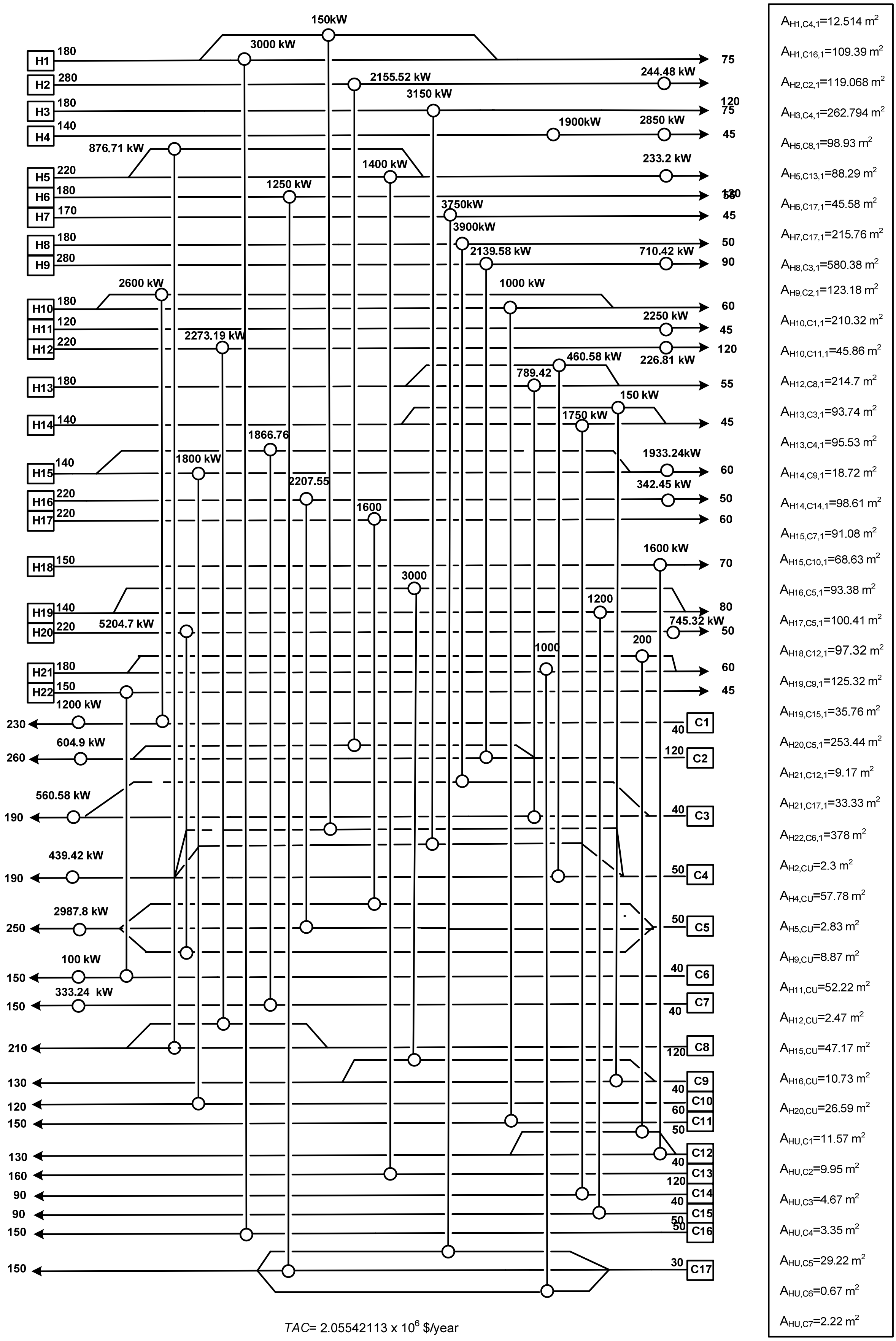


Figura 3A.12: HEN Configuration for the Case Study 05 using Synheat.

Chapter 4

Mixed-Integer Nonlinear Programming Models for Optimal Simultaneous Synthesis of Heat Exchangers Network

Abstract*: In this work the optimal simultaneous synthesis of heat exchanger networks is addressed. The model is based on a given stage wise superstructure and simultaneously minimizes the total annual cost as a result of the investment cost and operating costs in terms of energy consumption. Initially a general model is developed and then, this model is reduced to the Synheat model proposed by Yee and Grossmann (1990). The main idea is to compare the important features of Synheat Model. Three different case studies from literature are used to illustrate both models using the most common MINLP solvers, for which the computational performance is compared. This study shows the importance of proper assumptions in order to deal with the tradeoffs between model accuracy and quality and significance of the solution obtained with the model.*

**Published in the cyber infrastructure web site on MINLP (minlp.org) funded by the US-National Science Foundation. It consists in a virtual library of MINLP problems with the main goal of providing high level descriptions of the problems with one or several model formulations.*

4.1 Introduction

In this work we develop two models for the optimal simultaneous synthesis of heat exchanger networks based on a given stage wise superstructure. The objective is to find a network design that minimizes the total annualized cost in the design, i.e. the investment cost in units and the operating cost in terms of utility consumptions. The models simultaneously determine the number of units and size of the heat exchangers, as well the heating and cooling utility consumption. Two mixed-integer nonlinear programming (MINLP) formulations of this problem are presented. All mass and heat balances are performed, and also feasibility and logical constraints. The first formulation is a general straightforward nonconvex MINLP with a nonconvex objective function and several nonconvex constraints. In addition, it involves the logarithmic mean temperature that can result in numerical difficulties when the approach temperatures of both sides of the heat exchanger are equal (it can cause division by zero). The second formulation is the specialized MINLP model by Yee and Grossmann (1990) that is obtained assuming isothermal mixing of the streams in the superstructure, which significantly simplifies the model formulation, since nonlinear heat balances can be eliminated. For each stream, only an overall heat balance must be performed within each stage. Furthermore, the heat capacity flowrates are fixed, and hence flow variables are no longer needed in the model. In addition, the logarithmic mean temperature is replaced by the Chen approximation (Chen, 1987), where no logarithmic terms are involved. Moreover, the areas are not treated explicitly as a variable and its expressions are substituted in the objective function. As a result, not only the dimensionality of the problem is reduced, but the feasible space of the problem can be defined by a set of linear constraints. For this formulation, the nonlinearities are only involved in the objective function. When stream splits take place in the MINLP solution, an additional NLP model for fixed structure can be solved in order to remove the isothermal mixing assumption. Three examples are solved to illustrate the application of the models and compared their computational efficiency using MINLP solvers including Alpha-ECP, BARON, Bonmin, DICOPT and SBB.

4.2 Problem Statement

The optimal design of Heat Exchanger Networks addressed in this work can be stated as follows: Given a set of hot process streams $i \in HP$, which should be cooled from its inlet temperature $\left(T_i^{in}\right)$ to its outlet temperature (T_i^{out}); a set of cold process streams $j \in CP$, which should be heated from its inlet temperature $\left(T_j^{in}\right)$ to its outlet temperature $\left(T_j^{out}\right)$; the heat capacity flow rates of the hot (F_i^H) and cold process streams $\left(F_j^C\right)$; the utilities available (e.g., hot utilities HU and cold utilities CU) and their corresponding temperatures ($T_{CU}^{in}, T_{CU}^{out}$ and $T_{HU}^{in}, T_{HU}^{out}$) and costs ($c_{CU}$ and c_{HU}); Also given are the heat transfer coefficients for the hot streams h_i, for the cold streams h_j, and for the hot and cold utilities (h_{CU} and h_{HU}). Moreover, given are the fixed cost charge for each heat exchanger c_f and the coefficients α and β in order to calculate the cost of each heat exchanger according to its areas $\left(\alpha A^{\beta}\right)$. Given a staged superstructure as described in Yee and Grossmann (1990), the problem consists in finding the heat exchanger network with minimum annualized investment and operating costs, i.e. minimum Total Annualized Cost (TAC), by choosing the number of heat exchanger (n_U) and its respective areas (A), and the utility consumption levels $q_{CU,i}$ and $q_{HU,j}$.

4.3 General Model Formulation

The model formulation described here is based in a postulated stage-wise superstructure depicted in Figure 1 (Yee and Grossmann, 1990). The number of stages N_T, is normally set to $max\{N_H, N_C\}$, where N_H and N_C are the number of hot streams and the number of cold streams respectively. For each stage, the corresponding stream is split and directed to an exchanger for each potential match between each hot and each cold stream. The outlet temperatures are mixed, which then defines the stream for the next stage. The outlet temperatures of each stage are treated as variables in the formulation.

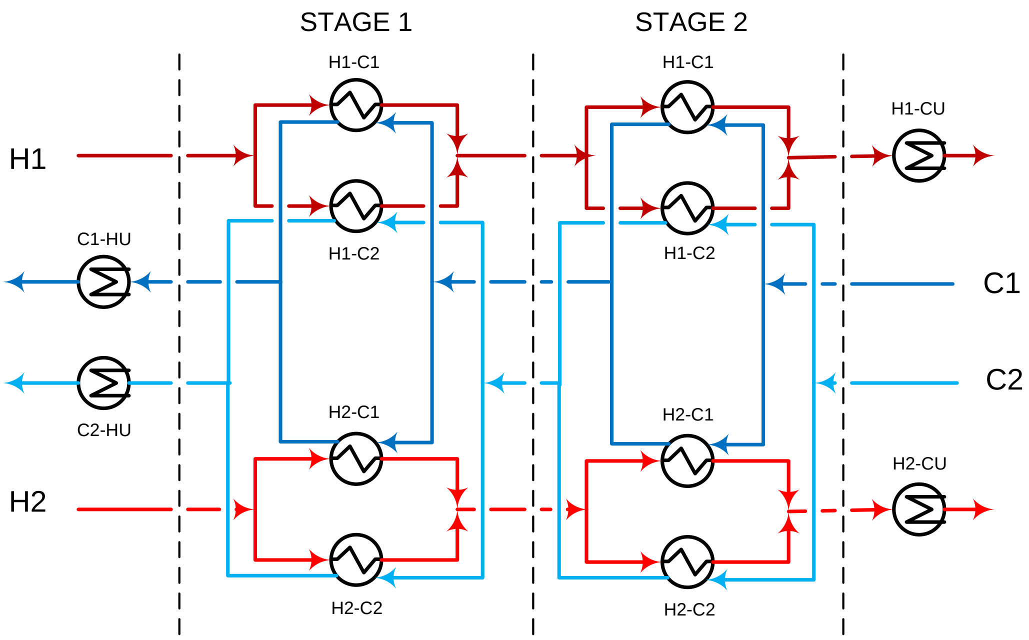


Figure 4.1: Two-stage Superstructure for two hot and two cold streams.

In the model formulation, an overall heat balance is needed to ensure sufficient heating or cooling of each process stream:

$$\sum_{k \in ST} \sum_{j \in CP} q_{ijk} + q_{cui} = F_i(T_i^{in} - T_i^{out}), i \in HP \tag{4.1}$$

$$\sum_{k \in ST} \sum_{i \in HP} q_{ijk} + q_{huj} = F_j(T_j^{out} - T_j^{in}), j \in CP \tag{4.2}$$

For each split, mass balances are performed to define the flowrates to each heat exchanger:

$$\sum_{j \in CP} f_{ijk}^H = F_i, i \in HP, k \in ST \tag{4.3}$$

$$\sum_{i \in HP} f_{ijk}^C = F_j, j \in CP, k \in ST \tag{4.4}$$

Energy balances around each heat exchanger are performed in order to define the outlet temperatures of heat exchanger, which leads to equations with bilinear terms:

$$q_{ijk} = f_{ijk}^{H}\left(t_{ik} - t_{ijk}^{H}\right), i \in HP, j \in CP, k \in ST \tag{4.5}$$

$$q_{ijk} = f_{ijk}^{C}\left(t_{jk+1} - t_{ijk}^{C}\right), i \in HP, j \in CP, k \in ST \tag{4.6}$$

Energy balances around each mixer define the inlet temperatures of the stages, which also involve bilinear terms:

$$F_i t_{ik+1} = \sum_{j \in CP} f_{ijk}^{H} t_{ijk}^{H}, i \in HP, j \in CP, k \in ST \tag{4.7}$$

$$F_j t_{jk} = \sum_{j \in CP} f_{ijk}^{C} t_{ijk}^{C}, i \in HP, j \in CP, k \in ST \tag{4.8}$$

According to the superstructure, the assignment of the inlet temperatures is as follows:

$$t_{i1} = T_i^{in}, i \in HP \tag{4.9}$$

$$t_{j,NT+1} = T_j^{in}, j \in CP \tag{4.10}$$

Energy balances for the final utility units define the utility loads:

$$q_{cui} = F_i\left(t_{i,NT+1} - T_i^{out}\right), i \in HP \tag{4.11}$$

$$q_{huj} = F_j\left(T_j^{out} - t_{j1}\right), j \in CP \tag{4.12}$$

The constraints (4.13) to (4.16) are used to ensure feasibility of temperatures. They specify monotonic decrease in the temperatures along the stages:

$$t_{ik+1} \le t_{ik}, i \in HP, k \in ST \tag{4.13}$$

$$t_{jk+1} \le t_{jk}, j \in CP, k \in ST \tag{4.14}$$

$$t_{iNT+1} \le T_i^{out}, i \in HP \tag{4.15}$$

$$t_{j1} \ge T_j^{out}, j \in CP \tag{4.16}$$

Upper bound constraints are needed to relate the heat loads q with the binary variables z. In the equations below Ω is an upper bound for the corresponding heat load. If the heat load is not equal to zero the corresponding binary variable is set to one, otherwise the binary variable can be 0 or 1, but the objective function forces the variable to be zero in order to minimize the number of units.

$$q_{ijk} - \Omega_{ij} z_{ijk} \leq 0, i \in HP, j \in CP, k \in ST \tag{4.17}$$

$$q_{cui} - \Omega_i z_{cui} \leq 0, i \in HP \tag{4.18}$$

$$q_{huj} - \Omega_j z_{huj} \leq 0, j \in CP \tag{4.19}$$

In addition, big-M constraints are needed to ensure that the temperature approaches only hold if the heat exchanger exists. The parameter Γ is an upper bound for the temperature difference. If the binary variable is equal to zero the equations are ensured to be feasible. On the other hand, if the binary variable is equal to one, the temperature differences are forced to act as an equality constraint in order to minimize the areas in the objective function.

$$dt_{ijk} \leq t_{ik} - t_{jk} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST \tag{4.20}$$

$$dt_{ijk+1} \leq t_{ik+1} - t_{jk+1} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST \tag{4.21}$$

$$dt_{cui} = t_{i,NT+1} - T_{out}^{CU} + \Gamma_i(1 - z_{cui}), i \in HP \tag{4.22}$$

$$dt_{huj} = T_{out}^{HU} - t_{i1} - T_{out}^{CU} + \Gamma_j\left(1 - z_{huj}\right), j \in CP \tag{4.23}$$

The trade-off between investment costs and operating costs are considered by adding the following constraints:

$$dt_{ijk} \leq \Delta T_{min}, i \in HP, j \in CP, k \in ST \tag{4.24}$$

$$dt_{cui} \leq \Delta T_{min}, i \in HP \tag{4.25}$$

$$dt_{huj} \leq \Delta T_{min}, j \in HP \tag{4.26}$$

The next equations are necessary to calculate the area of each unit. The driving forces are calculated by the logarithmic mean temperature difference for each heat exchanger:

$$LMTD_{ijk} = \frac{dt_{ijk} - dt_{ijk+1}}{\log\left(dt_{ijk}/dt_{ijk+1}\right)}, i \in HP, j \in CP, k \in ST \tag{4.27}$$

And the area of process-process heat exchangers can be calculated by the following equation:

$$A_{ijk} = q_{ijk}\left(h_i^{-1} + h_j^{-1}\right)/LMTD_{ijk}, i \in HP, j \in CP, k \in ST \tag{4.28}$$

Similarly for the utility exchangers, the temperature differences are calculated as follows:

$$LMTD_{cui} = \frac{dt_{cui} - \left(T_i^{out} - T_{CU}^{in}\right)}{\log\left(dt_{cui}/\left(T_i^{out} - T_{CU}^{in}\right)\right)}, i \in HP \tag{4.29}$$

$$LMTD_{huj} = \frac{dt_{huj} - \left(T_{HU}^{in} - T_j^{out}\right)}{\log\left(dt_{huj}/\left(T_{HU}^{in} - T_j^{out}\right)\right)}, j \in CP \tag{4.30}$$

And the areas of the utility units by the following equations:

$$A_{cui} = q_{cui}\,(h_i^{-1} + h_{CU}^{-1})/LMTD_{cui}\,, i \in HP \tag{4.31}$$

$$A_{huj} = q_{huj}\,\left(h_j^{-1} + h_{HU}^{-1}\right)/LMTD_{huj}\,, j \in CP \tag{4.32}$$

Finally, the objective function for the total annual cost (TAC) and the complete model are as follows:

$$\begin{aligned} TAC = min\, c_{CU} \sum_{i\in HP} q_{cui} + c_{HU} \sum_{j\in CP} q_{huj} \\ +c \sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} z_{ijk} + c \sum_{i\in HP} z_{cui} + c \sum_{j\in CP} z_{huj} \\ +\alpha \sum_{i\in HP}\sum_{j\in CP}\sum_{k\in ST} A_{ijk}^{\beta} + \alpha \sum_{i\in HP} A_{cui}^{\beta} + \alpha \sum_{j\in CP} A_{huj}^{\beta} \end{aligned} \tag{4.33}$$

The resulting MINLP model $(4.1) - (4.33)$ is nonconvex because the block of equations $(4.5) - (4.8)$ involve bilinear terms, and also the equations $(4.27) - (4.32)$ are non-linear and the objective function (4.33) is also nonlinear. In addition, the logarithmic mean temperature difference can cause numerical difficulties when driving forces are the same at both side of the heat exchanger, then LMTD reduces to zero by zero division, which is not determined.

4.4 Simplified Model Formulation (Yee and Grossmann, 1990)

In order to simplify the model, it is assumed that the outlet streams of each heat exchanger are mixed isothermically at each stage. For that special case, the energy balances around the mixers are no longer needed. For every hot and cold stream the outlet temperatures leaving the heat exchangers at the same stage k are to be the same, and they are associated with the downstream temperature location (t_{ik+1} for hot stream i and t_{jk} for cold stream j). In this way the energy balances for each hot and cold stream around each heat exchanger can be combined into overall heat balances per stage that are linear:

$$\sum_{j\in CP} q_{ijk} = F_i(t_{ik} - t_{ik+1}), i \in HP, k \in ST \tag{4.34}$$

$$\sum_{i \in HP} q_{ijk} = F_j\left(t_{jk} - t_{jk+1}\right), j \in CP, k \in ST \tag{4.35}$$

For the driving forces the logarithmic mean temperature difference for each heat exchanger is replaced by Chen approximation (1987):

$$LMTD_{ijk} = \left[dt_{ijk} dt_{ijk+1} \frac{dt_{ijk} + dt_{ijk+1}}{2}\right]^{1/3}, i \in HP, j \in CP, k \in ST \tag{4.36}$$

Similarly for the utility exchangers, the temperature differences are calculated as follows:

$$LMTD_{cui} = \left[dt_{cui}\left(T_i^{out} - T_{CU}^{in}\right) \frac{dt_{cui} + \left(T_i^{out} - T_{CU}^{in}\right)}{2}\right]^{1/3}, i \in HP \tag{4.37}$$

$$LMTD_{huj} = \left[dt_{huj}\left(T_{HU}^{in} - T_j^{out}\right) \frac{dt_{huj} + \left(T_{HU}^{in} - T_j^{out}\right)}{2}\right]^{1/3}, j \in CP \tag{4.38}$$

Finally, the objective function for the total annual cost TAC is the same way as expressed in equation (4.33), however, the areas in (4.28), (4.31) and (4.32) can be eliminated from the set of constraints if we replace the approximation (4.36) to (4.38) for the logarithmic mean temperature difference in the area definition, and the resulting expression can be substituted in the objective function. A similar procedure is used for the utility areas with which the objective function is rewritten as:

$$\begin{aligned} TAC = \min\ & c_{CU} \sum_{i \in HP} q_{cui} + c_{HU} \sum_{j \in CP} q_{huj} \\ & + c \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} z_{ijk} + c \sum_{i \in HP} z_{cui} + c \sum_{j \in CP} z_{huj} \\ & + \alpha \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} \left\{ \frac{\left(h_i^{-1} + h_j^{-1}\right) q_{ijk}}{\left[dt_{ijk} dt_{ijk+1} \frac{dt_{ijk} + dt_{ijk+1}}{2}\right]^{1/3}} \right\}^{\beta} \\ & + \alpha \sum_{i \in HP} \left\{ \frac{\left(h_i^{-1} + h_{CU}^{-1}\right) q_{cui}}{\left[dt_{cui}\left(T_i^{out} - T_{CU}^{in}\right) \frac{dt_{cui} + \left(T_i^{out} - T_{CU}^{in}\right)}{2}\right]^{1/3}} \right\}^{\beta} \\ & + \alpha \sum_{j \in CP} \left\{ \frac{\left(h_j^{-1} + h_{HU}^{-1}\right) q_{huj}}{\left[dt_{huj}\left(T_{HU}^{in} - T_j^{out}\right) \frac{dt_{huj} + \left(T_{HU}^{in} - T_j^{out}\right)}{2}\right]^{1/3}} \right\}^{\beta} \end{aligned} \tag{4.39}$$

It should be noticed that for the resulting MINLP the objective function in (4.39) subject to constraints (4.1), (4.2), (4.9) to (4.26), and (4.34), (4.35) the feasible space of the problem is defined by a set of linear constraints. The model, however is still nonconvex due to the nonlinearities involved in the objective function. Furthermore, numerical difficulties with the logarithmic mean temperature difference are overcome by the Chen approximation, which slightly overestimates the areas.

4.4.1 Nonlinear Programming Improvement Model

As pointed out before, when stream splits take place (i.e. a given stream has two or more exchangers at a given stage) an additional NLP model can be solved for further optimization in order to remove the isothermal mixing assumption by explicitly optimizing the outlet variables at the exchangers in which a split occurs.

For this problem the binary variables z_{ijk}, z_{cui} and z_{huj} are fixed and treated as parameters. For the NLP description some extra variables and parameters must be defined.

$Variables$	$Units$	
fh_{ijk}	$[kW/K]$	*heat capacity flowrate of heat exchanger between hot stream i and cold stream j at stage k*
fc_{ijk}	$[kW/K]$	*Heat capacity flow rate of heat exchanger between hot stream i and cold stream j at stage k*
t_{ijk}^{H}	$[K]$	*outlet temperature of the hot side of exchanger i, j, k*
t_{ijk}^{C}	$[K]$	*outlet temperature of the cold side of exchanger i, j, k*

$Binary\ Parameters$		
$z_{i,j,k}$	-	*existence of the match between hot stream i, cold stream j, at stage k*
z_{cui}	-	*existence of the match between hot stream i, and cold utility*
z_{huj}	-	*existence of the match between cold stream j, and hot utility*
y_{ik}	-	*existence of split for the hot stream i at stage k*
y_{jk}	-	*existence of split for the cold stream j at stage k*

Binary parameters are created to point out if some stream is split at stage k and they are defined by the following expressions:

$$if \sum_{j\in CP} z_{ijk} > 1; then\ y_{ik} = 1; else\ y_{ik} = 0$$

$$if \sum_{i\in HP} z_{ijk} > 1; then\ y_{jk} = 1; else\ y_{jk} = 0$$

The parameter y_{ik} is equal to one if the hot stream i is split at that stage k, and zero otherwise. Similarly the parameter y_{jk} is equal to one if the cold stream j is split at stage k. Based on these parameters extra expressions can be written. For each split, mass balances are performed to define the flowrates to each heat exchanger:

$$\sum_{j\in CP} f_{ijk}^{H} = F_i, i \in HP, k \in ST, y_{ik} = 1 \tag{4.40}$$

$$\sum_{i\in HP} f_{ijk}^{C} = F_j, j \in CP, k \in ST, y_{jk} = 1 \tag{4.41}$$

When a split occurs, energy balances around each heat exchanger are performed in order to define the outlet temperatures of heat exchanger:

$$q_{ijk} = f_{ijk}^{H}\left(t_{ik} - t_{ijk}^{H}\right), i \in HP, j \in CP, k \in ST, y_{ik} = 1 \tag{4.42}$$

$$q_{ijk} = f_{ijk}^{C}\left(tc_{jk+1} - t_{ijk}^{C}\right), i \in HP, j \in CP, k \in ST, y_{jk} = 1 \tag{4.43}$$

While energy balances around each mixer define the inlet temperatures of the stages:

$$F_i t_{ik+1} = \sum_{j \in CP} f_{ijk}^{H} t_{ijk}^{H}, i \in HP, j \in CP, k \in ST, y_{ik} = 1 \tag{4.44}$$

$$F_j t_{jk} = \sum_{j \in CP} f_{ijk}^{C} t_{ijk}^{C}, i \in HP, j \in CP, k \in ST, y_{jk} = 1 \tag{4.45}$$

Since the equations (4.40) to (4.45) only take place when the stream is split, we can define the outlet temperatures of the heat exchangers for the non-split stages as follows:

$$t_{ik+1} = t_{ijk}^{H}, i \in HP, j \in CP, k \in ST, y_{ik} = 0 \tag{4.46}$$

$$t_{jk} = t_{ijk}^{C}, i \in HP, j \in CP, k \in ST, y_{jk} = 0 \tag{4.47}$$

In addition, the logical constraints (4.17) and (4.18) must be rewritten according to the proper calculation of the driving forces for each heat exchanger:

$$dt_{ijk} \leq t_{ik} - t_{ijk}^{C} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST \tag{4.48}$$

$$dt_{ijk+1} \leq t_{ijk}^{H} - t_{jk+1} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST \tag{4.49}$$

The resulting NLP Improvement model can be defined as follows:

$$TAC = min\, c_{CU} \sum_{i \in HP} q_{cui} + c_{HU} \sum_{j \in CP} q_{huj} + c \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} z_{ijk} + c \sum_{i \in HP} z_{cui} + c \sum_{j \in CP} z_{huj} \quad + \alpha \sum_{i \in HP} \sum_{j \in CP} \sum_{k \in ST} \left\{ \frac{\left(h_i^{-1} + h_j^{-1}\right) q_{ijk}}{\left[dt_{ijk} dt_{ijk+1} \dfrac{dt_{ijk} + dt_{ijk+1}}{2}\right]^{1/3}} \right\}^{\beta}$$

$$+\alpha \sum_{i\in HP} \left\{ \frac{(h_i^{-1} + h_{CU}^{-1}) q_{cui}}{\left[dt_{cui}\left(T_i^{out} - T_{CU}^{in}\right) \frac{dt_{cui} + \left(T_i^{out} - T_{CU}^{in}\right)}{2} \right]^{1/3}} \right\}^{\beta}$$

$$+\alpha \sum_{j\in CP} \left\{ \frac{\left(h_j^{-1} + h_{HU}^{-1}\right) q_{huj}}{\left[dt_{huj}\left(T_{HU}^{in} - T_j^{out}\right) \frac{dt_{huj} + \left(T_{HU}^{in} - T_j^{out}\right)}{2} \right]^{1/3}} \right\}^{\beta}$$

$$s.t. \qquad (4.1) - (4.2), (4.9) - (4.16), (4.19) - (4.26), (4.34) - (4.35), (4.40) - (4.49)$$

The resulting model is a NLP since the binary variables z_{ijk}, z_{cui} and z_{huj} are fixed at their values defined by the solution of the previous MINLP step. In addition, according to the binary parameters y_{ik} and y_{jk}, the nonlinearities due to energy balances around each heat exchanger and mixer only take place for stages where some stream is split.

4.5 Numerical Examples

4.5.1 Example 1

The application of the general and the specialized models presented are illustrated first with a small example involving two hot streams and two cold streams; the number of stages considered is equal to two, and ΔT_{min} equals to 10. The input data of this example is given in Table 4.1.

Table 4.1: Problem data for Example 1 (Yee and Grossmann, 1990).

Stream	T_{in} (K)	T_{out} (K)	F (kW.K^{-1})	h (kW m^2 K^{-1})
H1	650	370	10	1
H2	590	370	20	1
C1	410	650	15	1
C2	350	500	13	1
CU	300	320		1
HU	680	680		5
Cost of Heat Exchangers (\$y^{-1}) = 5500+150[Area (m^2)]^1				
Cost of Cooling Utility = 15 (\$kW^{-1}y^{-1})				
Cost of Heating Utility = 80 (\$kW^{-1}y^{-1})				

The dimensions of the problems to be solved are presented in Table 4.2. The general model contains 12 binary variables and 113 continuous variables. The objective function is linear, since the exponent β is equal to one, and 48 of the 121 constraints in the model are nonlinear. On the other hand, the specialized model contains 12 binary variables and 57 continuous variables. The nonlinearities are only in the objective function, and the total number of linear constrains is 65. It should be noted that the number of continuous variables and the number of equations are almost 50% less than in the rigorous model.

Table 4.2: Models dimension for Example 1.

	General Model	*Specialized Model*
# binary variables	12	12
# continuous variables	113	57
# constraints	121	65
# nonlinear constraints	48	0

The continuous variables involved in both problems are positive. Upper bounds for the temperatures (as inlet temperatures for all hot temperatures, and outlet temperature for all cold temperatures), and upper bounds for flowrates at each stage (as the flowrates of the original stream) were also provided. The heat loads are bounded by the maximum heat exchange for each pair of streams, and the areas are bounded by the minimum driving force constraints. The initial values of all the variables are set to be on their lower bound, although other values can be specified. We tried to solve the general and the specialized models directly by using the Alpha-ECP 1.75.03, BARON 9.0.2, Coin-Bonmin 1.1, DICOPT 23.3.3 and SBB solvers with GAMS 23.3.3 on an Intel Core 2 Duo 2.13 GHz machine with 4 GB RAM.

The optimal objective function value, the total annual cost (TAC) calculated from the solution, and the computational time of each model are given in Table 4.3. Theoretically both models should give similar solutions, but as can be seen a much better solution was obtained with the specialized model. From the comparison, we can see that all solvers found the same optimal solution in the specialized model, but with different computational performance. Moreover, the solver DICOPT had the best performance followed by SBB and Bonmin. With the general model the solvers BARON and Bonmin were not able to find a feasible solution. AlphaECP obtained the best solution, while SBB and DICOPT converged faster but to a worst solution. It is clear that the solutions with the general model are highly suboptimal compared to the one of the specialized model.

Table 4.3: Results and Computational performance of the General and Specialized MINLP Models for the example problem 1.

Solver	*General Model*			*Specialized Model*		
	Obj. Function ($/year)	TAC ($/year)	CPU(s)	Obj. Function ($/year)	TAC ($/year)	CPU(s)
AlphaECP	300734.33	300740.14	3.258	154997.34	154910.97	11.65
Baron	*	*	*	154997.34	154892.97	284.66
Bonmin	*	*	*	154997.34	154892.97	3.05
SBB	396206.62	396137.90	0.165	154997.34	154892.97	3.03
DICOPT	396206.62	396137.90	0.267	154997.34	154892.97	0.30

**No feasible solution found*

The best solution found for the specialized model with all solvers has the objective value of 154997.34 \$/year and a correspondent Total Annual Cost of 154892.97 \$/year (where the areas are properly calculated with the logarithmic mean temperature difference). The best design is depicted in Figure 4.2. Since the design does not present stream splits, the isothermal mixing assumption is satisfied and the best solution found is also the best solution for the general model. However, it was not possible to find that solution with the general model.

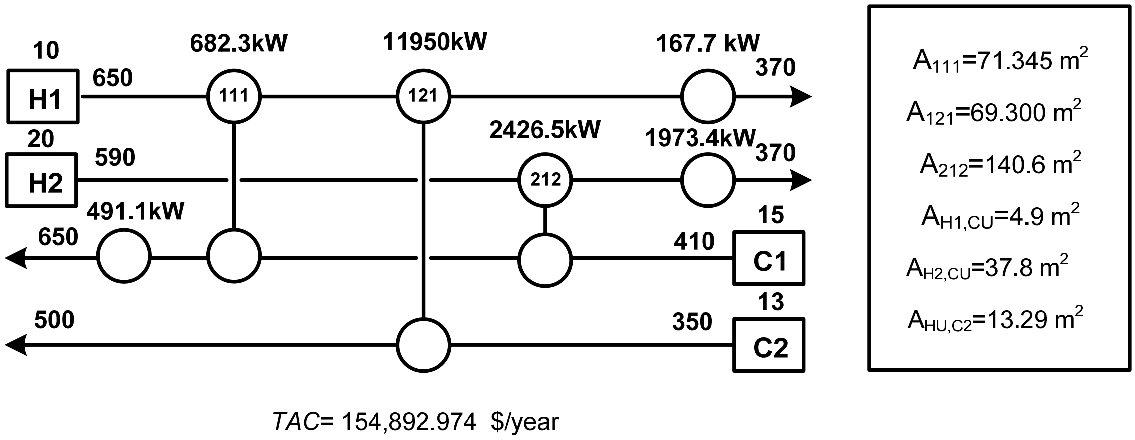


Figure 4.2: Heat Exchanger Network for Example 1.

4.5.2 Example 2

The second example presented consists of a problem with 5 hot streams and 1 cold stream; the number of stages selected is equal to 2[1], and $\Delta T_{\min}$ equals to 10 K. The input data of this example is given in Table 4.4.

Table 4.4: Problem data for Example 2 (Yee and Grossmann, 1990).

Stream	T_{in} (K)	T_{out} (K)	F (kW.K^{-1})	h (kW m^2 K^{-1})
H1	500	320	6	2
H2	480	380	4	2
H3	460	360	6	2
H4	380	360	20	2
H5	380	320	12	2
C1	290	660	18	2
CU	300	320		1
HU	700	700		2

Cost of Heat Exchangers (\$y^{-1}) = 5500+1200[Area (m^2)]$^{0.6}$
Cost of Cooling Utility = 10 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 140 (\$kW^{-1}y^{-1})

As seen in Table 4.5 the general model contains 21 binary variables and 200 continuous variables. The objective function is nonlinear, since β is equal to 0.6, and 97 of the 226

[1] We obtained the same results with 3 stages, and one of them was in fact empty, i.e. no matches taking place.

constraints in the model are nonlinear. The simplified model contains 21 binary variables and 98 continuous variables. The nonlinearities are only in the objective function, and the total number of linear constrains is 118.

Tabela 4.5: Models dimension for Example 2.

	General Model	*Specialized Model*
# binary variables	21	21
# continuous variables	200	98
# constraints	226	118
# nonlinear constraints	97	0

Providing the bounds as in example 1 and setting the initial values at their lower bounds, we tried to solve both models directly. The results and computational performance are presented in Table 4.6.

Tabela 4.6: Results and Computational performance of the General and Specialized MINLP Models for the example problem 2.

Solver	*General Model*			*Specialized Model*		
	Obj. Function ($/year)	TAC ($/year)	CPU(s)	Obj. Function ($/year)	TAC ($/year)	CPU(s)
AlphaECP	834701.97	833173.916	2.481	1032138.78	1032138.78	1.372
Baron	*	*	*	637415.28	637278.43	3600
Bonmin	*	*	*	*	*	*
SBB	739019.02	737942.94	0.234	634979.34	634849.12	0.718
DICOPT	833733.41	832656.14	2.172	634979.34	634849.12	0.227

**No feasible solution found*

For this example, even for the specialized model we had different performances. The MINLP solvers DICOPT and SBB presented higher performance and robustness. BARON reached the maximum time provided of one hour but it converged to a slightly suboptimal solution. For the general model, when the solvers were able to find a solution, they converged to a worse suboptimal solution compared with the specialized model. It is interesting to note that for the general model the MINLP solver SBB presented the best performance.

The best solution found, for the specialized model with the solvers SBB and DICOPT has the objective value of 634979.34 $/year and a corresponding Total Annual Cost of 634849.12 $/year. The best design is depicted in Figure 4.3. For this example there are some splits and hence the isothermal mixing assumption is used for the mixed streams. Since in the MINLP solution some streams are mixed isothermically, an NLP for fixed structure can be solved in order to remove the isothermal mixing assumption as seen in Figure 4.4, we can observe a slight reduction in the objective function (less than 1 %), showing that the isothermal mixing assumption is quite good.

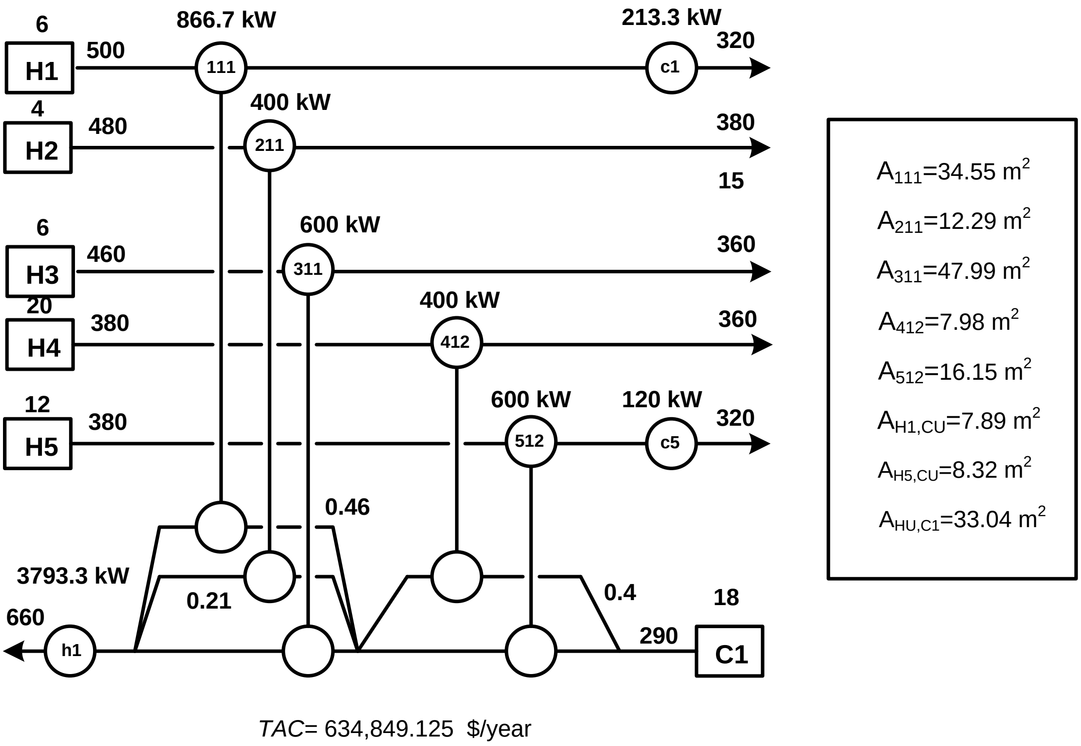


Figure 4.3: Heat Exchanger Network for Example 2 from the MINLP solution.

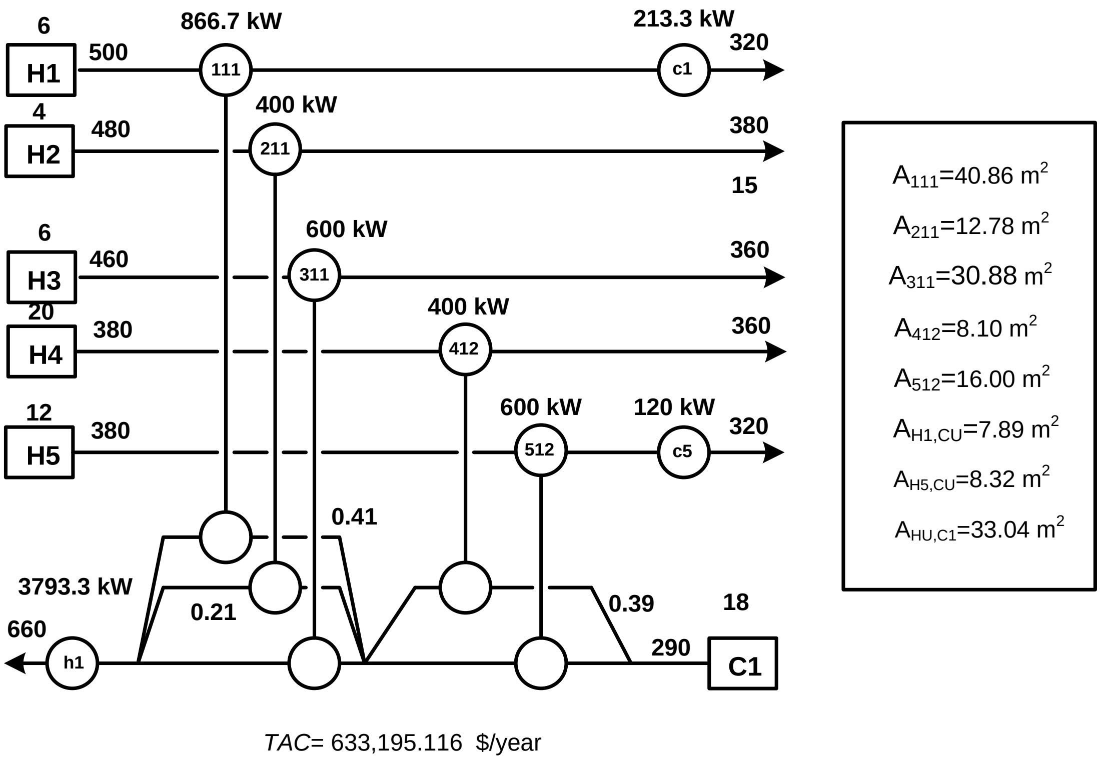


Figure 4.4: Heat Exchanger Network for Example 2 with NLP improvement.

4.5.3 Example 3

The third example consists of a problem with 5 hot streams and 5 cold streams; the number of stages selected is equal to 2[2], and ΔT_{min} equals to 10. The input data of this example is given in Table 4.7. As seen in Table 8, the general model contains 60 binary variables and 581 continuous variables. The objective function is nonlinear, since β is equal to 0.6, and 88 of the 511 constraints in the model are nonlinear. The specialized model contains 60 binary variables and 261 continuous variables. The nonlinearities are only in the objective function, and the total number of linear constrains is 251.

Table 4.7: Problem data for Example 3 (Chakraborty and Ghoshb, 1999).

Stream	T_{in} (°C)	T_{out} (°C)	F (kW°C^{-1})	h (kW m^2 °C^{-1})
H1	160	93.3	8.8	1.7
H2	248.9	137.8	10.6	1.7
H3	226.7	65.6	14.8	1.7
H4	271.1	148.9	12.6	1.7
H5	198.9	65.6	17.7	1.7
C1	60	160	7.6	1.7
C2	115.6	221.7	6.1	1.7
C3	37.8	221.1	8.4	1.7
C4	82.2	176.7	17.3	1.7
C5	93.3	204.4	13.9	1.7
CU	25	40		1.7
HU	240	240		3.4

Cost of Heat Exchangers (\$y^{-1}) = 4000+146[Area (m^2)]$^{0.6}$
Cost of Cooling Utility = 10 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 200 (\$kW^{-1}y^{-1})

Table 4.8: Models dimension for Example 3.

	General Model	*Specialized Model*
# binary variables	60	60
# continuous variables	581	261
# constraints	511	251
# nonlinear constraints	88	0

We tried to solve both models directly. The results and computational performance are presented in Table 4.9. The best solution found for the specialized model was again obtained with the MINLP solvers SBB and DICOPT. BARON reached the time limit obtaining a suboptimal solution and the solvers AlphaECP and Bonmin were not able to find solutions. The general model was only solved with the solver SBB, converging to a highly suboptimal solution if compared with the specialized model.

[2] We obtained a similar analysis with 3 stages. There is no significant improvement in terms of solution and it is computationally more expensive.

Table 4.9: Results and Computational performance of the General and Specialized MINLP Models for the example problem 3.

Solver	General Model			Specialized Model		
	Obj. Function ($/year)	TAC ($/year)	CPU(s)	Obj. Function ($/year)	TAC ($/year)	CPU(s)
AlphaECP	**	**	**	**	**	**
Baron	**	**	**	68612.22	68671.29	3600
Bonmin	*	*	*	*	*	*
SBB	228070.41	227368.97	5.335	64937.23	64930.51	14.35
DICOPT	***	***	***	64937.23	64930.51	0.227

No feasible solution found; * *No solution returned ;* No integer solution found.*

The best solution found, for the specialized model with the solvers SBB and DICOPT has the objective value of 64937.23 $/year and a corresponding Total Annual Cost of 64930.51 $/year. The best design is depicted in Figure 4.5. For this example there are some splits and hence the isothermal mixing holds for the mixed streams. The NLP improvement model was used to remove the isothermal mixing assumption, which provided a small improvement of less than 1 %, as seen in Figure 4.6.

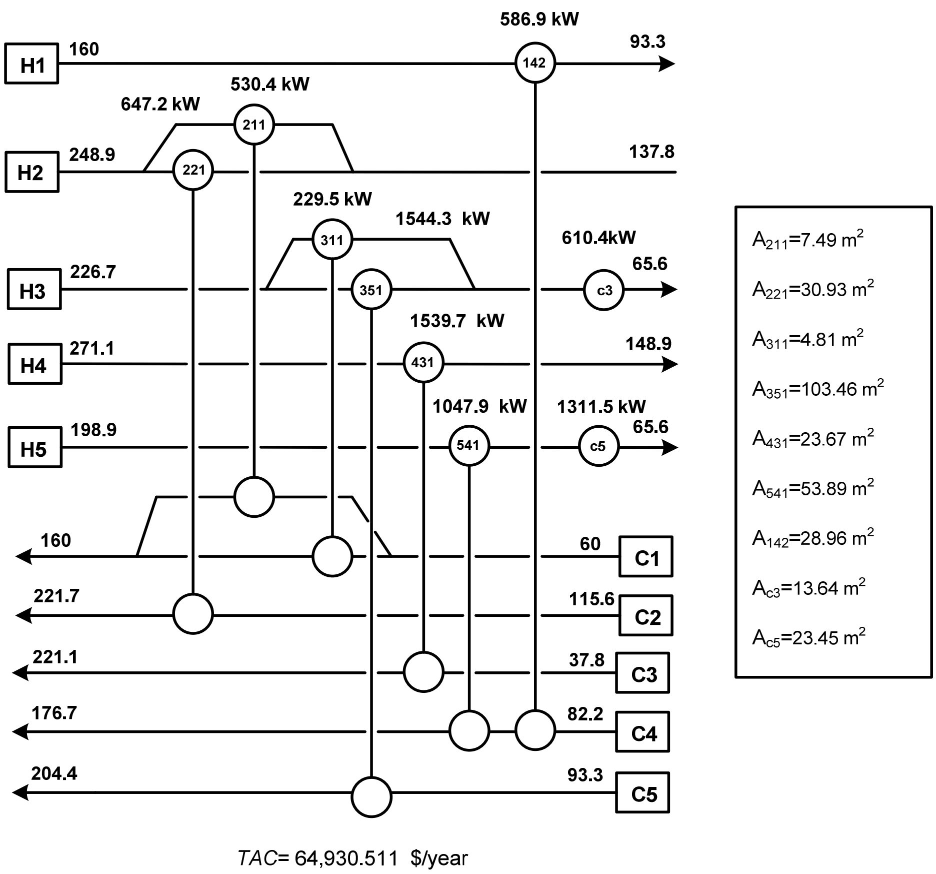


Figure 4.5: Heat Exchanger Network for Example 3 from the MINLP solution.

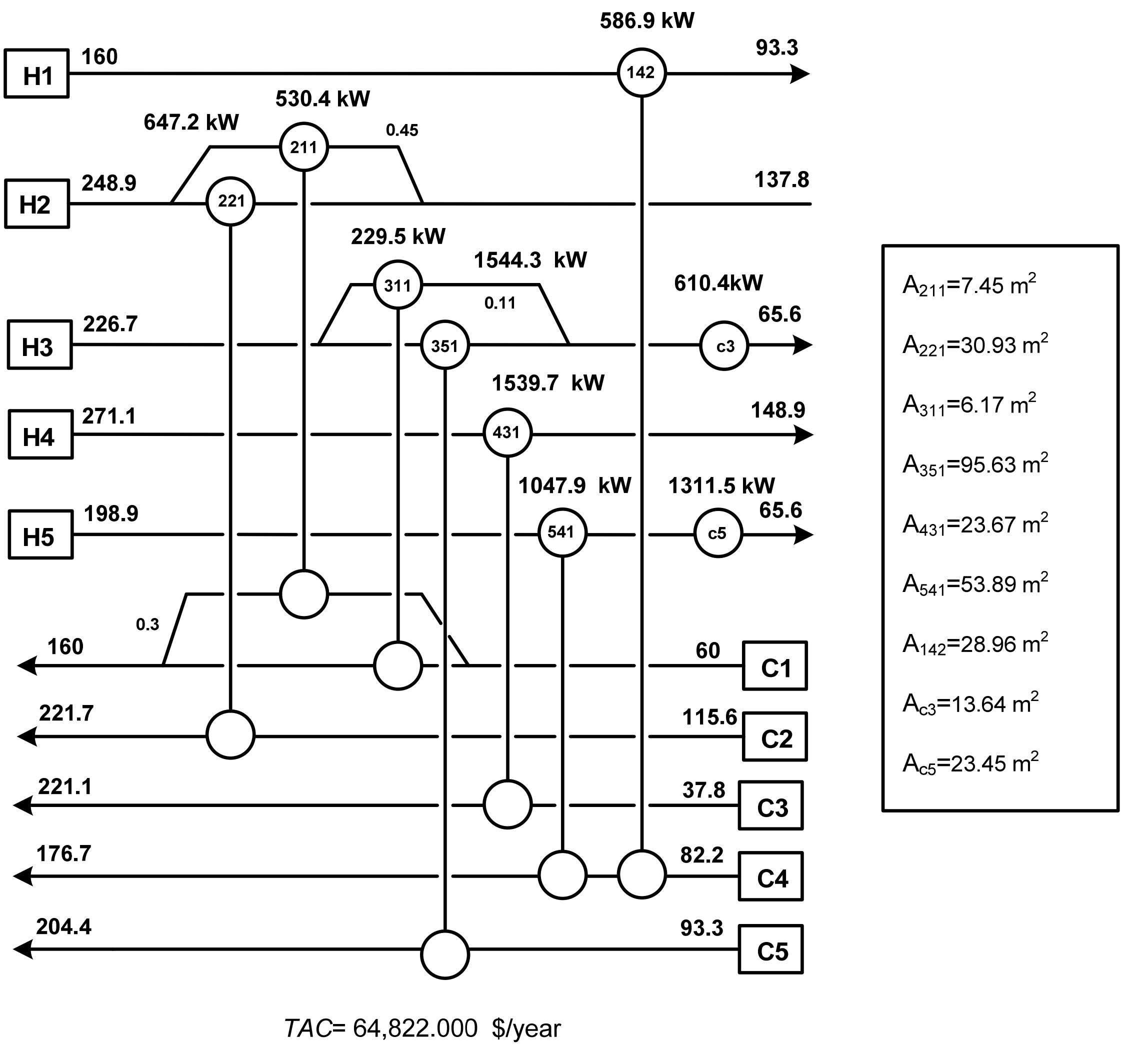


Figure 4.6: Heat Exchanger Network for Example 3 NLP improvement.

4.5.4 On the Initial Values

It is clear that the specialized model is easier to solve, and even with the isothermal mixing assumption, it is possible to find the best solutions. One question that may arise is whether it is possible to provide a good initial guess to the general model. We should note that the solution obtained with the specialized model is a feasible solution for the general case. We tested this idea for providing a good initial guess for the general case. The results obtained are presented in Table 4.10.

For the example 1 we can realize an improvement in the solution found when compared with the previous results for the general case. In the best case, the solver Bonmin finds essentially the best solution, which however in not better compared to the specialized model. For the second and third case studies the initialization with the specialized model does not improve the solution, and for the third case study the solution obtained with the initial guess is in fact better.

Table 4.10: Results and Computational performance of the General MINLP Model using the solution of Specialized MINLP Model as initial guess for the example problem 1, 2, and 3.

	Example 1		*Example 2*		*Example 3*	
Solver	Obj. Function ($/year)	CPU(s)	Obj. Function ($/year)	CPU(s)	Obj. Function ($/year)	CPU(s)
AlphaECP	193955.95	3.716	835281.01	2.780	**	**
Baron	*	*	*	*	*	*
Bonmin	154895.93	98.55	*	*	*	*
SBB	155399.86	1.614	1033371.69	0.062	77755.86	24.43
DICOPT	212216.19	0.606	1033371.69	0.062	**	**

4.6 General Remarks and Conclusions

The specialized model represents a simplified version of the general case. The interesting feature of this model is that it is smaller in terms of number of equations and number of continuous variables and also the feasible region is defined by a set of linear constraints. It makes the problem easier and more robust to solve. Three case studies were presented showing that specialized model formulation is more computationally efficient in terms of quality of solution obtained and robustness. For some instances the general model was faster to solve but normally converging to highly suboptimal solutions. If we try to solve the general model without using any strategy to obtain a good initial value, it is usually not possible to obtain a good solution. Even giving a good initial guess for the general model, obtained from the specialized model, it was not possible to find better or even good solutions with the general case.

In addition, we should point out that the MINLP solvers SBB and DICOPT in general had the best computational performances in the sense of time consumption and quality of solution obtained. An important point to be considered is that when the solution obtained with the MINLP specialized model present splits, an additional NLP model can be performed for fixed structure in order to remove the isothermal mixing assumption by explicitly optimizing the outlet variables at the exchangers in which a split occurs. It was showed that despite the fact that the isothermal mixing assumption restricts the search space is not that bad assumption. For thermodynamic reasons, mixing streams with very different temperatures is not thermally efficient.

The main lesson of this problem is the great importance of problem reformulation. Modeling the problem rigorously, it is possible to obtain an accurate model, but if we do not have a good strategy to solve the problem, we may not obtain good solutions. Making good assumptions in order to simplify the problem to be solved is clearly a crucial point. Finally, both models with documentation, discussion and GAMS files for each numerical example have been available at http://minlp.org/library/problem/index.php?i=93&lib=MINLP, where is possible to find a virtual library of problems in different application areas in which one or several alternative models are presented with their derivation

Nomenclature

Sets	
CP	*set of cold process stream j*
CU	*set of cold utility*
HP	*set of hot process stream i*
HU	*set of hot utility*
ST	*set of stages in the superstructure*

Parameters	*Units*	
α	$[\$/yr]$	*factor for the area cost*
β	-	*exponent for the area cost*
c	$[\$/yr]$	*fixed charge for exchangers* ($/year)
c_{CU}	$[\$/kW.yr]$	*utility cost coefficient for cooling utility j*
c_{HU}	$[\$/kW.yr]$	*utility cost coefficient for heating utility i*
F_i	$[kW/K]$	*flow capacity of hot stream i*
F_j	$[kW/K]$	*flow capacity of cold stream j*
h_i	$[kW/m^2K]$	*heat transfer coefficient for hot stream i*
h_j	$[kW/m^2K]$	*heat transfer coefficient for cold stream j*
h_{CU}	$[kW/m^2K]$	*heat transfer coefficient for cold utility*
h_{HU}	$[kW/m^2K]$	*heat transfer coefficient for cold utility*
N_T	-	*number of stages*
T_i^{in}	$[K]$	*inlet temperature of hot stream i*
T_j^{in}	$[K]$	*inlet temperature of cold stream j*
T_i^{out}	$[K]$	*outlet temperature of hot stream i*
T_j^{out}	$[K]$	*outlet temperature of cold stream j*
Ω	$[kW]$	*upper bound for heat exchangers loads*
Γ	[^{o}C]	*upper bound for temperature difference*

Positive Variables	*Units*	
A_{ijk}	$[m^2]$	*heat load between hot stream i and cold stream j at stage k*
A_{cui}	$[m^2]$	*heat load between hot stream i and cold utility*
A_{huj}	$[m^2]$	*heat load between cold stream j and hot utility*
fh_{ijk}	$[kW/K]$	*flow rate of heat exchanger between hot stream i and cold stream j at stage k*
fc_{ijk}	$[kW/K]$	*flow rate of heat exchanger between hot stream i and cold stream j at stage k*

th_{ik}	$[K]$	*temperature of hot stream i at hot end of stage k*
tc_{jk}	$[K]$	*temperature of cold stream j at hot end of stage k*
t_{ijk}^{H}	$[K]$	*outlet temperature of the hot side of exchanger i, j, k*
t_{ijk}^{C}	$[K]$	*outlet temperature of the cold side of exchanger i, j, k*
dt_{ijk}	$[K]$	*temperature approach between hot stream i, cold stream j, at location k*
dt_{cui}	$[K]$	*temperature approach between hot stream i, and cold utility*
dt_{huj}	$[K]$	*temperature approach between cold stream j, and hot utility*
$LMTD_{i,j,k}$	$[K]$	*log mean temperature difference between hot stream i, cold stream j, at stage k*
$LMTD_{cui}$	$[K]$	*log mean temperature difference between hot stream i, and cold utility*
$LMTD_{huj}$	$[K]$	*log mean temperature difference between cold stream j, and hot utility*
q_{ijk}	$[kW]$	*heat load between hot stream i and cold stream j at stage k*
q_{cui}	$[kW]$	*heat load between hot stream i and cold utility*
q_{huj}	$[kW]$	*heat load between cold stream j and hot utility*
t_{ik}	$[K]$	*temperature of hot stream i at hot end of stage k*
t_{jk}	$[K]$	*temperature of cold stream j at hot end of stage k*

$Binary\ Variables$

$z_{i,j,k}$	-	*existence of the match between hot stream i, cold stream j, at stage k*
z_{cui}	-	*existence of the match between hot stream i, and cold utility*
z_{huj}	-	*existence of the match between cold stream j, and hot utility*

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Chapter 5

A Lagrangean Heuristic Approach for Multiperiod Heat Exchanger Network Synthesis

***Abstract**: In this work we apply a decomposition technique to address the multiperiod heat exchanger network synthesis. Each period correspond to periodical changes in operating conditions, i.e. inlet temperatures and flowrates. The problem size grows quickly with the number of streams and the number of periods resulting in a large scale problem to solve. In order to reduce the problem to a manageable size we proposed a specialized heuristic algorithm that relies on the concept of Lagrangean decomposition. We present an iterative scheme where feasible solutions are postulated from the Lagrangean decomposition subproblems, and multipliers are updated through a subgradient method. Three numerical examples are used to illustrate the proposed approach and the obtained solutions were compared with the full space solutions, i.e. with no decomposition. In general, slightly better suboptimal solutions were found but in the terms of computational efforts its use is only justified as we increased the problem size.*

Proposed Outlet: Computers and Chemical Engineering.

5.1 Introduction

Heat Exchanger Network Synthesis (HENS) is an important part in the overall chemical process. From the energy point of view we can see an overall process system as three main interactive components (Figure 5.1), which can be integrated into an operable plant (Aaltola, 2002).

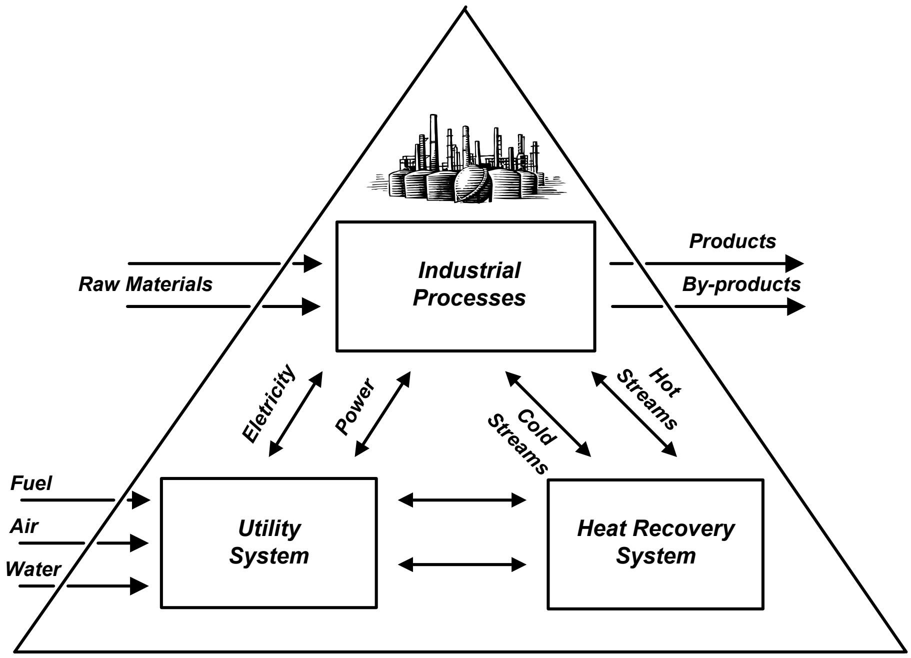

Figure 5.1: *An overall process system.*

The design of the HEN links the process flowsheet with the utility system and generally involves a large fraction of both, the overall plant capital cost, and operating costs in terms of energy requirements being a key factor for a profitable process (Verheyen e Zhang, 2006).

The conventional Heat Exchanger Network Synthesis is performed under the assumption of fixed operating parameters at nominal conditions for a given specification of a process design. The major techniques are based on sequential (Linnhoff and Hindmarsh, 1983; Papoulias and Grossmann, 1983; Floudas et al., 1986) and simultaneous approaches (Ciric and Floudas, 1991; Yee and Grossmann, 1990), for a recent review see the paper by Furman and Sahinidis, 2002.

In practice, the operating conditions are expected to change due to variations normally encountered, i.e. uncertainty. Uncertainty is an inherent characteristic of any chemical processes. They may have different sources such as: (*i*) unknown disturbances like uncertainty in the process parameters (operating conditions); (*ii*) uncertain model parameters (kinetic parameters, heat transfer coefficients, etc); (*iii*) discrete uncertainty (failures, equipment availability, etc). Plant flexibility has been recognized to represent one of the important components in the operability of the production process, since it is related to the capability of a process to achieve feasible operation over a given range of uncertain conditions (Grossmann e Floudas, 1987).

The incorporation of uncertainty into design may be possible through a deterministic approach based on the postulation of a finite number of periods (scenarios) to characterize the uncertainty and the problem can be formulated as multiscenario/multiperiod optimization problem. The solution of the multiperiod design problem can be embedded in a two stage strategy in order to generate flexible heat exchanger networks. The main limitation consists in the muitliperiod problem dimension, which may be large with the number of streams and the number of periods. On the other hand, multiperiod problems present a block diagonal structure, which can be exploited using decomposition techniques.

The focus in this work is in the multiperiod problem formulation for Heat Exchanger network synthesis and its decomposable structure. This chapter is organized as follows: the Section 5.2 provides a literature review while the Section 5.3 presents the mathematical formulation of the problem. The outline of the proposed method is sketched in Section 5.4 and some numerical examples are presented in Section 5.5. Finally, conclusions and final remarks are given in Section 5.6.

5.2 Literature Review

Operability issues are very important for heat integrated process, since the economic performance of a process is greatly affected by process variations and the ability of the system to satisfy its operational specifications under external disturbances or inherent modeling uncertainty. The ability of the plant to handle process parameter changes on steady state operation is regarded as process flexibility. Several authors have developed systematic methods for the synthesis of HENs, which are flexible to operate under uncertain conditions and operable for disturbances. A general overview with the main remarkable works is sketched in Figure 5.2.

The work of Marselle et al. (1982) was a pioneer in operability considerations for heat exchanger networks. They firstly developed the concept of resilient HENs, which can tolerate uncertainties in temperatures and flowrates. This method, however, needs a manual combination of a series of optimal designs under different worst-case scenarios, making the application of this method to large-size problems practically impossible.

In order to measure the degree of flexibility of a HEN, Saboo et al. (1985) proposed the Resilience Index (RI). The RI characterizes the largest total uncertainty which a HEN can tolerate while remaining feasible. The RI can be used to compare different options on a quantitative basis. Swaney and Grossmann (1985) introduced a Flexibility Index (FI), which represents a maximum deviation of an uncertain parameter while still remaining within the feasible region. The Flexibility Index provides a basis for different designs to be compared as well as providing the necessary information about which critical points in the feasible region limit the design. At that moment, the proposed algorithms to compute the Flexibility Index relied on assumptions that made the problem tractable only for the case where the constraints were convex.

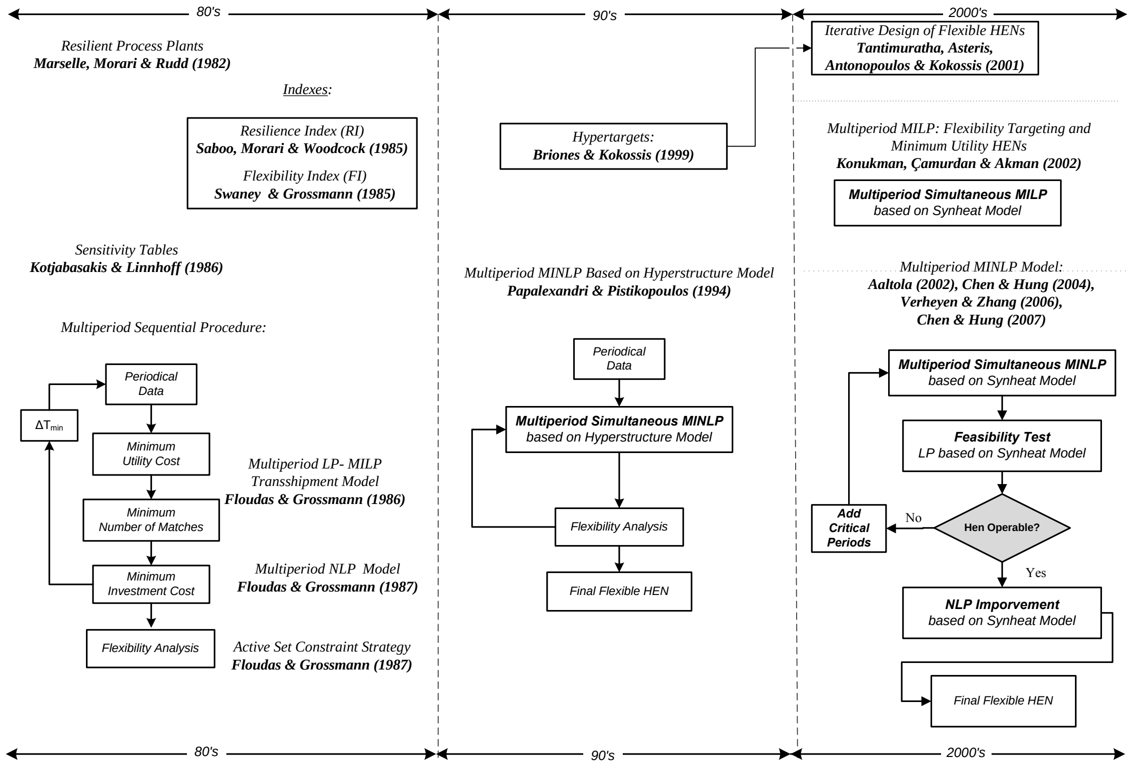

Figure 5.2: General Overview on methods for Design of Flexible HENs.

Kotjabasakis and Linnhoff (1986) introduced the sensitivity tables for the design of flexible HENs. They developed a method to find which heat exchanger areas should be increased and which heat exchanger should be bypassed in order to make a nominal design sufficiently flexible. In this work disturbances are assessed and the nominal design is modified to be able to handle those. Finally the design may be verified prior to realization through dynamic simulation of the open and closed loop system.

Grossmann and Floudas (1987) introduced an active set strategy for automated solution of the Flexibility Index of Swaney and Grossmann (1985). The solution approach was used to circumvent the previous limitation, and the resulting MI(N)LP formulation can be used to nonconvex constraints.

Tantimuratha et al. (2000) proposed a two-stage design procedure, where the first stage consists of area targeting using the hypertarget model developed by Briones and Kokossis (1999). For a selected set of matches from the first stage, the network is optimized with an iterative procedure to minimize annual costs. The method proposed can be used in both grassroots and retrofit cases. This method, however, could still lead to suboptimal solutions because it relies on decomposition.

Multiperiod HEN design

It is very common to represent the uncertainty as a discrete set of operating conditions, for which a multiperiod problem is formulated. For HENs, different formulations have been proposed in the literature. Floudas and Grossmann (1987) proposed a sequential HEN synthesis method that combines the multiperiod mixed-integer linear programming (MILP) transshipment with the active set strategy to guarantee the desired HEN flexibility. They first introduced a multiperiod MILP model based on the transshipment model of Papoulias and Grossmann (1983). This model determines the minimum utility consumption and minimum number of matches through the pinch points at each operating period. The next stage is a reformulated NLP model that develops the network configuration. Here again, the decomposition of the problem into different stages significantly reduces the size of the problem, but does not take into account the tradeoffs between area, number of units, and energy rigorously.

Papalexandri and Pistikopoulos (1994) presented a framework for the synthesis and retrofit of flexible and structurally controllable HENs considering HEN synthesis and flexibility simultaneously using mathematical programming in a large MINLP problem. This of course, limits the size of the problem to relatively small scale problems. The algorithm is based on a multiperiod hyperstructure network representation, where explicit structural controllability criteria are developed and included in a MINLP model. As point out by Mathisen (1994), this formulation yields a very complex model and the solution to the simple examples presented are not convincing.

The most recent developments for simultaneous synthesis for flexible HENs are based on the stage-wise superstructure presentation and an isothermal mixing assumption of Yee and Grossmann (1990). The assumptions in the original formulation make the constraint set linear and hence very attractive for robustness on the solution using the current available algorithms. The next approaches described here are based on SYNHEAT model. Konukman et al. (2002) presented a MILP model, which introduces simultaneous flexibility targeting and the synthesis of the minimum utility heat exchanger networks. The formulation presumes that the feasible region in the space of input parameters is convex; therein the optimal solution is explored on the basis of the vertices of the polyhedral region of uncertainty. It limits the applicability only for uncertainty in the inlet temperatures. Furthermore, the investment cost is not considered explicitly in the formulation, but only by the limitation of the driving forces to avoid large areas. The formulation is solved successively, for increasing values of the target flexibility, to reveal the necessary structural modifications and their corresponding utility consumption level.

Aaltola (2002) proposed a model which simultaneously optimizes the multiperiod MINLP problem for minimum costs and flexibility, without relying on sequential decomposition. In the model proposed by Aaltola, it was avoided explicit modeling of bypasses in the MINLP model, which would introduce non-linear constraints into the set of constraints. The objective function considers the area of one match to be the mean value of areas in different periods, and therefore there is an underestimation of the total area cost and the Total Annual Cost (TAC). He reasoned that the introduction of maximum area into the formulation would introduce nonlinearities into the set of constraints or nonlinearities with discontinuous derivatives into the objective function.

Chen and Hung (2004) proposed a three-step approach for designing flexible multiperiod HENs, which is based on the stage-wise HEN superstructure representation of Yee and Grossmann and the mathematical formulation of Aaltola. The authors introduced the maximum area consideration in the objective function and decomposed the problem into three main iterative steps: simultaneous HEN synthesis, flexibility analysis, and removal of infeasible networks using integer cuts. The number of iterations required in this approach is of concern for industrial problems. Chen and Hung (2004) considered the issue of a maximum area in their formulation by using the discontinuous function “max”, which results in more expensive computation.

Verheyen and Zhang (2006) combined the advantages of both approaches Konukman, Çamurdan et al. (2002) and Aaltola (2002). They proposed that the calculation of maximum area can be achieved by allowing more nonlinear inequalities into the set of constraints. The new equations limit the new variable (installed area) to be greater than or equal of the required are for each period, and the minimization of the objective function will push the areas toward its minimum possible value, which is the maximum required area per period.

Chen and Hung (2007) proposed a simulation based strategy for simultaneous synthesis of heat exchanger networks. They used the same mathematical multiperiod formulation than Verheyen and Zhang (2006) aborting their previous discontinuous formulation. They also try to avoid the tedious mathematical analysis in the flexibility test, and a simplified test is applied for a big number of simulations where the various inputs conditions are generated randomly within the operational range. The most violating point is considered as an additional period. The simplified test is made without considering the restraints on unit sizes, and the resulting test is a LP problem. An additional step requires the resizing of exchangers to guarantee the flexible operation over the whole disturbance range when a NLP is solved.

Recently, the multiperiod formulations for HENs are based on the simultaneous approach proposed by Yee and Grossmann (1990). In the next section this model and its extension for multiperiod representation are presented.

5.3 Mathematical Formulation

The model ($P1$) consists in the original SYNHEAT model proposed by (Yee and Grossmann, 1990). This model is obtained assuming isothermal mixing of the streams, which significantly simplifies the model formulation. The stage wise superstructure is depicted in Figure 2. In this formulation nonlinear heat balances can be eliminated. For each stream, only an overall heat balance must be performed within each stage. Furthermore, the heat capacity flowrates are fixed, and hence flow variables are no longer needed in the model. In addition, the logarithmic mean temperature is replaced by the Chen approximation (Chen, 1987), where no logarithmic terms are involved.

Moreover, the areas are not treated explicitly as a variable and are substituted in the objective function. As a result, not only the dimensionality of the problem is reduced, but the feasible space of the problem can be defined by a set of linear constraints. For this formulation, the nonlinearities are only involved in the objective function. These characteristic make the Synheat model very attractive to work. As pointed out in the previous section multiperiod formulation has been used to address the flexibility on HEN design. The MINLP problem ($P1$) was extended by different authors in the literature for multiperiod representation. In general, this extension is very straightforward regarding the design variables as invariant for all periods, while the state variables and control variables (degrees of freedom) are allowed to vary for different realization of uncertain parameters (periods). Here the design variables are the installed area of each heat exchanger and the binary variables denoting the existence of the matches. The general form of the multiperiod optimization problem for HENS are described in model ($P2$), while the objective function for different formulations are listed in Table 5.1.

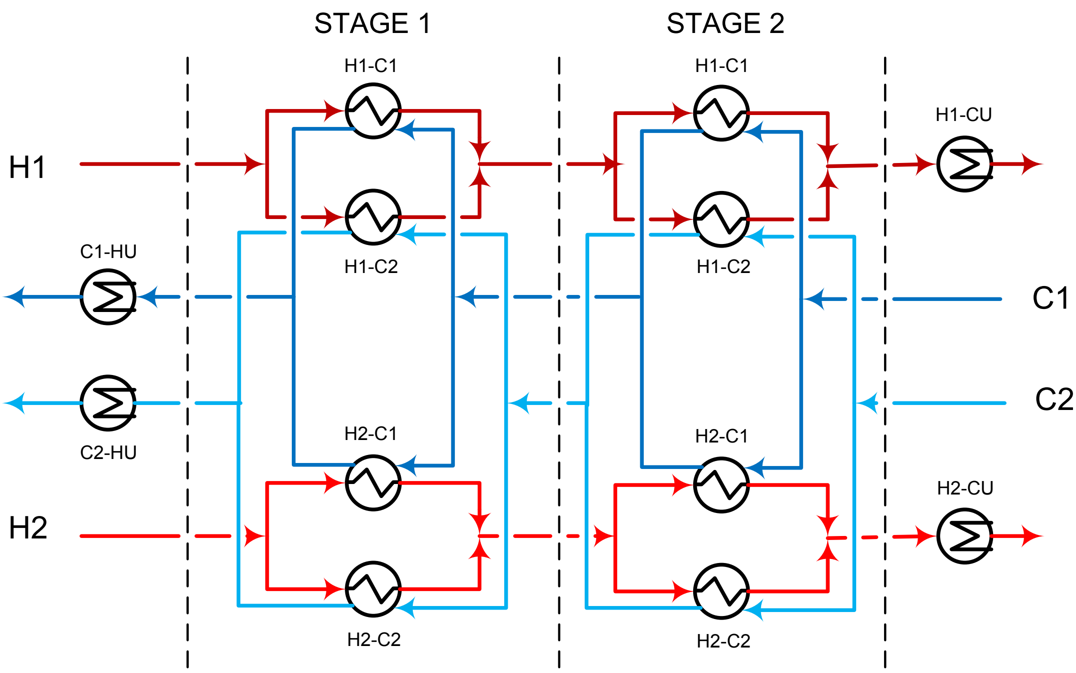

Figure 5.3: Superestructure for Synheat Model (Yee and Grossman, 1990) exemplified for two hot streams, to cold streams and two stages.

The multiperiod formulations for simultaneous synthesis of flexible HENs based on SYNHEAT model mainly differ in objective function $J^p(x)$. The upperscript p points out the corresponding variable in period p. The parameter $DOP(p)$ corresponds to the duration of the period, which is difficult to determine accurately, in general, it is assumed the same duration for each period. It should be noticed that in the formulations presented the bypass are not explicitly modeled, as a consequence the area must vary to represent the bypass effect. In practice, the installed area of heat exchanger area will be unique. It is rather obvious that if we have a different required area for each period, the maximum one must be selected as installed area. Afterwards a bypass must be placed across the heat exchanger, and the other operating periods can be physically achieved by bypass manipulations. The nominal bypass value may be calculated in a straightforward manner. However the tricky question is how to compute the correct investment cost, since the installed area must be considered in its estimation and a priori we do not know for which period the maximum area will occur.

$$\text{Synheat MINLP Model}$$

$$\min_{x\in\Omega}\left\{\begin{array}{c}\sum_{i\epsilon HP} c_{cu}q_{cui} + \sum_{j\epsilon CP} c_{hu}q_{huj} + \\ \sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} cf_{ijk}z_{ijk} + \sum_{i\epsilon HP} cf_{cu}z_{cui} + \sum_{j\epsilon CP} cf_{hu}z_{huj} + \\ \sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} c_{ij}\left(\frac{q_{ijk}}{U_{ij}LMTD_{ijk}}\right)^{\beta} + \sum_{i\epsilon HP} c_{cui}\left(\frac{q_{cui}}{U_{cui}LMTD_{cui}}\right)^{\beta} + \sum_{j\epsilon CP} c_{huj}\left(\frac{q_{huj}}{U_{huj}LMTD_{huj}}\right)^{\beta}\end{array}\right\}$$

$$x = \left\{\begin{array}{c} z_{ijk}, z_{cui}, z_{huj}; \\ t_{ik}, t_{jk}; \\ dt_{ijk}, dt_{cui}, dt_{huj}; \\ q_{ijk}, q_{cui}, q_{huj}; \\ \forall i \in HP, j \in CP, k \in ST \end{array}\right\}$$

$$\Omega = \left\{\begin{array}{c}
\left.\begin{array}{c}(T_i^{in} - T_i^{out})w_i = \sum_{\forall k\in ST}\sum_{\forall j\in CP} q_{ijk} + q_{cui} \\ (T_j^{out} - T_j^{in})w_j = \sum_{\forall k\in ST}\sum_{\forall j\in HP} q_{ijk} + q_{huj}\end{array}\right\} \begin{array}{c}\text{overall} \\ \text{heat balance}\end{array} \\
\left.\begin{array}{c}(t_{ik} - t_{i,k+1})w_i = \sum_{\forall j\in CP} q_{ijk} \\ (t_{jk} - t_{j,k+1})w_j = \sum_{\forall i\in HP} q_{ijk}\end{array}\right\} \begin{array}{c}\text{stagewise} \\ \text{heat balances}\end{array} \\
\left. t_{i1} = T_i^{in}\ ,\ \ t_{j,N_T+1} = T_j^{in} \right\} \begin{array}{c}\text{assignment of} \\ \text{inlet temperature}\end{array} \\
\left.\begin{array}{c} t_{ik} \geq t_{i,k+1}\ ,\ \ t_{jk} \geq t_{j,k+1} \\ T_i^{out} \leq t_{i,N_T+1}\ ,\ \ T_j^{out} \geq t_{j1}\end{array}\right\} \begin{array}{c}\text{feasibility of} \\ \text{temperature}\end{array} \\
\left.\begin{array}{c}(t_{i,N_T+1} - T_i^{out})w_i = q_{cui} \\ (T_j^{out} - t_{j1})w_j = q_{huj}\end{array}\right\} \text{utility loads} \\
\left.\begin{array}{c} q_{ijk} - \Lambda_{ij}z_{ijk} \leq 0 \\ q_{cui} - \Lambda_i z_{cui} \leq 0 \\ q_{huj} - \Lambda_j z_{huj} \leq 0\end{array}\right\} \begin{array}{c}\text{logical} \\ \text{constraints}\end{array} \\
\left.\begin{array}{c} dt_{ijk} \leq t_{ik} - t_{jk} + \Gamma_{ij}(1 - z_{ijk}) \\ dt_{ij,k+1} \leq t_{i,k+1} - t_{j,k+1} + \Gamma_{ij}(1 - z_{ijk}) \\ dt_{cui} \leq t_{i,N_T+1} - T_{cu}^{out} + \Gamma_i(1 - z_{cui}) \\ dt_{huj} \leq T_{hu}^{out} - t_{j1} + \Gamma_j(1 - z_{huj})\end{array}\right\} \begin{array}{c}\text{approach} \\ \text{temperatures}\end{array} \\
dt_{ijk}, dt_{cui}, dt_{huj} \geq \Delta T_{min} \\
z_{ijk}, z_{cui}, z_{huj} \in \{0,1\} \\
q_{ijk}, q_{cui}, q_{huj} \geq 0 \\
\forall i \in HP, j \in CP, k \in ST
\end{array}\right\} \qquad (P1)$$

$$\mathit{Synheat\ Multiperiod\ MINLP\ Model}$$
$$\min_{x\in\Omega}\{J^p\}$$

$$x = \left\{ \begin{array}{c} z_{ijk}, z_{cui}, z_{huj}; \\ t_{ik}^p, t_{jk}^p; \\ dt_{ijk}^p, dt_{cui}^p, dt_{huj}^p; \\ q_{ijk}^p, q_{cui}^p, q_{huj}^p; \\ \forall i \in HP, j \in CP, k \in ST, p \epsilon PR \end{array} \right\}$$

$$\Omega = \left\{ \begin{array}{ll}
\left.\begin{array}{c} \left(T_i^{in,p} - T_i^{out}\right) w_i^p = \sum\limits_{\forall k\in ST} \sum\limits_{\forall j \in CP} q_{ijk}^p + q_{cui}^p \\ \left(T_j^{out,p} - T_j^{in,p}\right) w_j^p = \sum\limits_{\forall k\in ST} \sum\limits_{\forall i \in HP} q_{ijk}^p + q_{huj}^p \end{array}\right\} & \begin{array}{c} \mathit{overall} \\ \mathit{heat\ balance} \end{array} \\
\left.\begin{array}{c} \left(t_{ik}^p - t_{i,k+1}^p\right) w_i^p = \sum\limits_{\forall j\in CP} q_{ijk}^p \\ \left(t_{jk}^p - t_{j,k+1}^p\right) w_j^p = \sum\limits_{\forall i\in HP} q_{ijk}^p \end{array}\right\} & \begin{array}{c} \mathit{stagewise} \\ \mathit{heat\ balances} \end{array} \\
t_{i1}^p = T_i^{in,p}, \quad t_{j,N_T+1}^p = T_j^{in,p} \Big\} & \begin{array}{c} \mathit{assignment\ of} \\ \mathit{inlet\ temperature} \end{array} \\
\left.\begin{array}{c} t_{ik}^p \ge t_{i,k+1}^p, \quad t_{jk}^p \ge t_{j,k+1}^p \\ T_i^{out,p} \le t_{i,N_T+1}^p, \quad T_j^{out,p} \ge t_{j1}^p \end{array}\right\} & \begin{array}{c} \mathit{feasibility\ of} \\ \mathit{temperature} \end{array} \\
\left.\begin{array}{c} \left(t_{i,N_T+1}^p - T_i^{out,p}\right) w_i^p = q_{cui}^p \\ \left(T_j^{out,p} - t_{j1}^p\right) w_j = q_{cui}^p \end{array}\right\} & \mathit{utility\ loads} \\
\left.\begin{array}{c} q_{ijk}^p - \Lambda_{ij} z_{ijk} \le 0 \\ q_{cui}^p - \Lambda_i z_{cui} \le 0 \\ q_{huj}^p - \Lambda_j z_{huj} \le 0 \end{array}\right\} * & \begin{array}{c} \mathit{logical} \\ \mathit{constraints} \end{array} \\
\left.\begin{array}{c} dt_{ijk}^p \le t_{ik}^p - t_{jk}^p + \Gamma_{ij}\left(1 - z_{ijk}\right) \\ dt_{ij,k+1}^p \le t_{i,k+1}^p - t_{j,k+1}^p + \Gamma_{ij}\left(1 - z_{ijk}\right) \\ dt_{cui}^p \le t_{i,N_T+1}^p - T_{cu}^{out,p} + \Gamma_i\left(1 - z_{cui}\right) \\ dt_{cui}^p \le T_{hu}^{out,p} - t_{j1}^p + \Gamma_j\left(1 - z_{huj}\right) \end{array}\right\} * & \begin{array}{c} \mathit{approach} \\ \mathit{temperatures} \end{array} \\
dt_{ijk}^p, dt_{cui}^p, dt_{huj}^p \ge \Delta T_{min} & \\
z_{ijk}, z_{cui}, z_{huj} \in \{0,1\} & \\
q_{ijk}^p, q_{cui}^p, q_{huj}^p \ge 0 & \\
\forall i \in HP, j \in CP, k \in ST, p \in PR &
\end{array} \right\} \qquad (P2)$$

Table 5.1: Objective function for different multiperiod formulations based on Synheat Model.

(i) -(Konukman, Çamurdan et al., 2002)

$$\min_{x\in\Omega}\left\{\sum_{p\in PR}\left(\sum_{i\epsilon HP} c_{cu} q_{cui}^{p} + \sum_{j\epsilon CP} c_{hu} q_{huj}^{p}\right)\right\}$$

(ii) Formulation 1:-(Aaltola, 2002)

$$\min_{x\in\Omega}\left\{\begin{array}{c}\displaystyle\sum_{p\in PR}\frac{DOP(p)}{N_P}\left(\sum_{i\epsilon HP} c_{cu} q_{cui}^{p} + \sum_{j\epsilon CP} c_{hu} q_{huj}^{p}\right) + \\ \displaystyle\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} cf_{ijk} z_{ijk} + \sum_{i\epsilon HP} cf_{cu} z_{cui} + \sum_{j\epsilon CP} cf_{hu} z_{huj} + \\ \displaystyle\sum_{p\in PR}\frac{1}{N_P}\left(\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} c_{ij}\left(\frac{q_{ijk}^{p}}{U_{ij} LMTD_{ijk}^{p}}\right)^{\beta} + \sum_{i\epsilon HP} c_{cui}\left(\frac{q_{cui}^{p}}{U_{cui} LMTD_{cui}^{p}}\right)^{\beta} + \sum_{j\epsilon CP} c_{huj}\left(\frac{q_{huj}^{p}}{U_{huj} LMTD_{huj}^{p}}\right)^{\beta}\right)\end{array}\right\}$$

(iii) (Chen and Hung, 2004)

$$\min_{x\in\Omega}\left\{\begin{array}{c}\displaystyle\frac{1}{N_P}\left(\sum_{i\epsilon HP} c_{cu} q_{cui}^{p} + \sum_{j\epsilon CP} c_{hu} q_{huj}^{p}\right) + \\ \displaystyle\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} cf_{ijk} z_{ijk} + \sum_{i\epsilon HP} cf_{cu} z_{cui} + \sum_{j\epsilon CP} cf_{hu} z_{huj} + \\ \displaystyle\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} c_{ij}\left[max\left(\frac{q_{ijk}^{p}}{U_{ij} LMTD_{ijk}^{p}}\right)\right] + \sum_{i\epsilon HP} c_{cui}\left[max\left(\frac{q_{cui}^{p}}{U_{cui} LMTD_{cui}^{p}}\right)\right] + \sum_{j\epsilon CP} c_{huj}\left[max\left(\frac{q_{huj}^{p}}{U_{huj} LMTD_{huj}^{p}}\right)\right]\end{array}\right\}$$

(ii) Formulation 2: −(Verheyen and Zhang, 2006), (Chen and Hung, 2007)

$$\min_{x\in\Omega'}\left\{\begin{array}{c}\displaystyle\sum_{p\in PR}\frac{DOP(p)}{N_P}\left(\sum_{i\epsilon HP} c_{cu} q_{cui}^{p} + \sum_{j\epsilon CP} c_{hu} q_{huj}^{p}\right) + \\ \displaystyle\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} cf_{ijk} z_{ijk} + \sum_{i\epsilon HP} cf_{cu} z_{cui} + \sum_{j\epsilon CP} cf_{hu} z_{huj} + \\ \displaystyle\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} c_{ij}\left(A_{ijk}\right)^{\beta} + \sum_{i\epsilon HP} c_{cui}\left(A_{cui}\right)^{\beta} + \sum_{j\epsilon CP} c_{huj}\left(A_{huj}\right)^{\beta}\end{array}\right\}$$

$$\Omega' = \Omega \cup \left\{\begin{array}{l} A_{ijk} \geq \dfrac{q_{ijk}^{p}}{U_{ij} LMTD_{ijk}^{p}} \\ A_{cui} \geq \dfrac{q_{cui}^{p}}{U_{cui} LMTD_{cui}^{p}} \\ A_{huj} \geq \dfrac{q_{huj}^{p}}{U_{huj} LMTD_{huj}^{p}}\end{array}\right\}$$

Different approaches have been developed: Aaltola (2002) considered the varying area and the average area in the objective function to overcome this problem. Chen and Hung, (2004) used the discontinuous function "max" resulting in a discrete objective function. Verheyen and Zhang (2006) proposed the use of inequalities to provide an upper bound on this area at cost of adding nonlinearities in the set of constraints. The model of Konukman, et al. (2002) does not face this problem, because it does not consider the area in the formulation. As a result despite the robustness this model underestimates the investment costs and may result in large areas. One interesting point that seems to be neglected is that the multiperiod problem can be large. On the other hand, multiperiod problems present a special structure, which can be exploited by decomposition techniques. In this work we consider the formulation of Aaltola (2002) and the formulation of Verheyen and Zhang (2006), for further investigation, since they are the most promising.

5.4 Outline of the Solution Strategy

The multiperiod models such as (*P2*) grow quickly in size with the number of periods N, making it very difficult to solve them without the help of specialized techniques (Karuppiah and Grossmann, 2008). Moreover, multiperiod design problems present an interesting block diagonal structure that can be exploited. Generally we have a subset of constraints that holds for each period and a subset of constraints holding for all periods, regarded as linking constraints. In fact, the multiperiod SYNHEAT model is linked by the design variables (z_{ijk} and A_{ijk}), which can be easily reformulated in terms of linking constraints. In order to solve the problem for large scale instances we propose using Lagrangean Decomposition, which is coupled with a heuristic technique in order to generate a sequence of upper and lower bounds.

5.4.1 Lagrangean Decomposition

The problem of muliperiod synthesis of heat exchanger network based on SYNHEAT model (*P2*) can be written in the following way:

$$(P): \left\{ \begin{array}{c} z_P = \min_{x^p,y} f(x^p) + c^T y \\ s.t. \begin{array}{c} h(x^p) = 0 \\ g(x^p) \leq 0 \end{array} \\ Ax^p + By \leq 0 \ * \end{array} \right\} \tag{5.1}$$

where x^p are the continuous variables and y the binary variables. The corresponding inequalities were marked with a star (*) in model (P) and model (*P2*). The binary variables are regarded as complicating variables in the sense that they link the periods preventing a straightforward solution. However, this problem can be reformulated as a problem with complicating constraints if we split the complicating variables into periods $\{y^1, \ldots, y^N\}$ and in order to ensure the equivalence to the original problem, non-anticipativity constraints are added $\{y^1 = \cdots = y^N\}$ resulting in the following problem, which is equivalent to (P):

$$(P'): \left\{ \begin{array}{c} z_{P'} = \min_{x^p,y} f(x^p) + c^T \sum_{p=1}^{N} y^p / N \\ s.t. \begin{array}{c} h(x^p) = 0 \\ g(x^p) \leq 0 \end{array} \\ Ax^p + By^p \leq 0 \\ y^p - y^{p+1} = 0 \,, p = 1 \ldots N-1 \end{array} \right\} \tag{5.2}$$

The model (P') can be decomposed removing the non-anticipativity constraints from the constraint set by the concept of Lagrangean decomposition (Guignard and Kim, 1987). Initially, the problem (P') is relaxed removing the copy constraints from the set of constraints by dualization, i.e. adding in the objective function multiplied by the Lagrangean multipliers $\mu^p\left(y_{ijk}^p - y_{ijk}^{p'}\right)$ resulting in the model (LD_μ). This model yields a decomposable problem into N subproblems, whose solution provides a lower bound for the unknown optimal value of (P), i.e. the original multiperiod problem.

$$(LD_\mu):\left\{\begin{array}{c} z_{LD} = \min_{x^p,y^p} f(x^p) + c^T \sum_{p=1}^{N} y^p/N + \mu^p(\, y^p - y^{p+1}) \\ s.t.\ \begin{array}{c} h(x^p) = 0 \\ g(x^p) \le 0 \end{array} \\ Ax^p + By^p \le 0 \end{array}\right\} \tag{5.3}$$

The set of constraints of the problem described in (5.3) are independent in terms of periods and hence this problem can be solved independently by the solution of N subproblems. Each subproblem can be written as follows:

$$(SP_p):\left\{\begin{array}{c} z_{SP} = \min_{x^p,y^p} f(x^p) + c^T \sum_{p=1}^{N} y^p/N + y^p(\, \mu^p - \mu^{p-1}) \\ s.t.\ \begin{array}{c} h(x^p) = 0 \\ g(x^p) \le 0 \end{array} \\ Ax^p + By^p \le 0 \end{array}\right\} \tag{5.4}$$

where $\mu^0 = \mu^N = 0$. Solving each subproblem for a given set of Lagrangean multipliers μ^p yields a valid lower bound $z_{LB}^{\mu} = z_{LD} = \sum_{p=1}^{N} z_{SP_p}^*$ for the original problem. An interesting point to be considered is that the dimension of each subproblem is equivalent to the dimension for the conventional design considering only nominal conditions. It makes the problem tractable independent of the number of periods, once we are able to solve the problem for a given realization of uncertain parameters. Solving the Lagrangean dual problem (LD_μ) in the dual space by searching for a best set of Lagrangean multipliers, provides the tightest lower bound:

$$z_{LB} = \max_{\mu}\left(LD_\mu\right) \tag{5.5}$$

Since this dual problem is non differential and difficult to solve directly. Here we use the subgradient method (Held and Karp, 1970; Held et al., 1974) where we iterate with different values of the Lagrange multipliers according to the formula :

$$\mu^{p,k+1} = \mu^{p,k} + \lambda^k\left(Z_{UB}^k - Z_{LB}^k\right)(y^{p,k} - y^{p+1,k})/\|y^{p,k} - y^{p+1,k}\|^2 \tag{5.6}$$

where $\lambda^k \in [0,2]$ is a scalar used to control the step size in the dual space. This value can be reduced if no improvement is found for a certain number of iterations. This method is easy to implement and very often used. In order to apply the subgradient method, we need an estimative of an upper bound at each iteration. One could postulate a feasible solution of the original problem. Fixing the set of binary variables and solving the original MINLP problem as a NLP, if a feasible solution is obtained this solution is an upper bound for the original problem. In this work the solution of the subproblems are combined in order to postulate a feasible solution for the original problem. The proposed procedure can be described as follows:

Postulating a Feasible Solution

1. Solve decomposed dual subproblems for fixed multipliers;
2. If $z_{ijk}^{p} = 0 \ \forall \ p$, then fix z_{ijk}^{p} to zero;
   If $z_{ijk}^{p} \neq 0 \ \forall \ p$, then $z_{ijk}^{p} \in M$
3. Solve the Multiperiod problem in the reduced space:
   $$\left\{\begin{matrix} min_{z \in M} \sum_i \sum_j \sum_k m_{ijk} + c_{cu}/p \sum_p \sum_i q_{cui} + c_{hu}/p \sum_p \sum_j q_{huj} \\ m_{ijk} \geq \sum_p z_{ijk}^{p} \ ; \ \Omega(p) \end{matrix}\right\}$$
4. Fix the solution obtained z_{ijk}^{p} and solve the Multiperiod NLP model to obtain the upper bound.

For the sake of simplicity, we considered the binary variables as the complete set, i.e. $z_{ijk}^{p} = \{z_{ijk}^{p}, z_{cui}^{p}, z_{huj}^{p}\}$. The overall procedure is depicted in Figure 5.4. Initially, all the Lagrangean multipliers are fixed to zero and then, each subproblem as in (5.4) is solved for each problem. The summation of objective functions provides the current lower bound. A feasible set of binary variables is postulated according to the procedure described and the original MINLP problem is solved as a NLP to generate an Upper bound. The set of Lagrangean multipliers is updated according to the formula (5.6). The procedure terminates if the duality gap (difference between the upper and lower bounds) is small or if the maximum number of iterations is reached and the best feasible solution (upper bound) is reported.

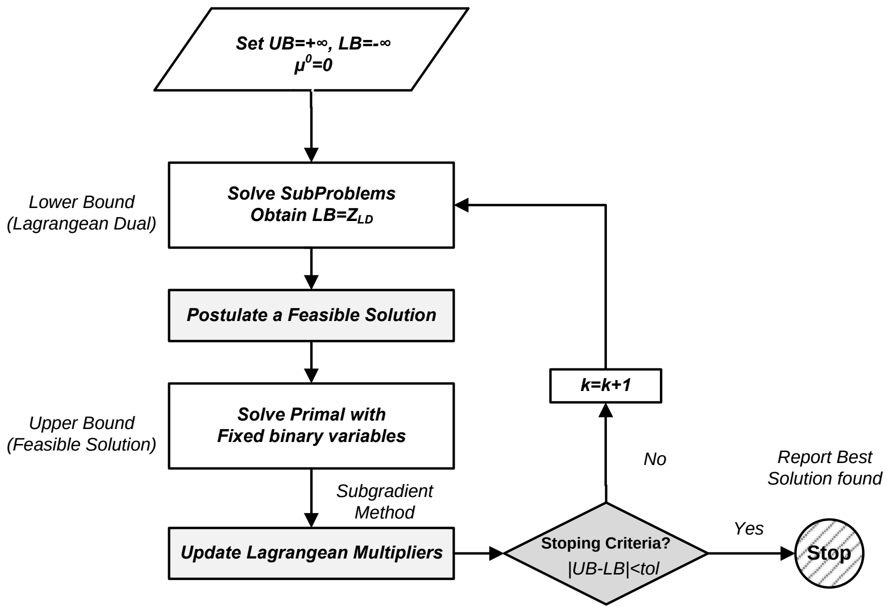

Figure 5.4: Lagrangean Heuristic Approach for solving multiperiod Synheat model.

5.5 Numerical Examples

Three illustrative examples of simultaneous synthesis of multiperiod heat exchanger networks were solved. The MINLP models were formulated using GAMS and solve on an Intel Core i5 2.67 GHz machine with 2.96 GB memory. GAMS/CONOPT 3.0 was used to solve the NLP problems, GAMS/CPLEX 10.0 was used for the MILP problems, and GAMS/DICOPT was employed for solving the MINLP problems. For the generation of scenarios /periods we use the critical scenarios identified by Marselle et al. (1982), assuming expected variations of δ from nominal condition in positive and negative directions.

Table 5.2: Nominal and Critical Periods for Synthesis of Heat exchanger networks.

Case	*Stream Type*	*Inlet Temperature Variations*	*Flow rate Variation*	*Description*
1	Hot	0	0	Nominal
	Cold	0	0	
2	Hot	-	+	Min ΔT
	Cold	+	+	Max Area
3	Hot	-	-	Max Heat
	Cold	-	+	
4	Hot	+	+	Max Cooling
	Cold	+	-	

5.5.1 Numerical Example 01

The first numerical example involves two hot streams and two cold streams. The nominal data for the problem is listed in Table 5.3. It is expected variations in the inlet temperatures of $\delta_T = 10K$ and a variation of $\delta_F = 10\%$ in the heat capacity flowrates. The minimum number of stages was set to two.

Table 5.3: Problem data for Example 01.

Stream	T_{in} (ºC)	T_{out} (ºC)	*F* (kWºC^{-1})	*h* (kW m^2 ºC^{-1})
H1	650	370	10	1
H2	590	370	20	1
C1	410	650	15	1
C2	350	500	13	1
CU	300	320		1
HU	680	680		5

Cost of Heat Exchangers (\$y^{-1}) = 5500+150[Area (m^2)]^1
Cost of Cooling Utility = 15 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 80 (\$kW^{-1}y^{-1})

The example was solved for the nominal data using the Synheat Model and solved using Formulation1 proposed by Aaltola (2002) appending new periods according to the Table 5.2. The cost data, i.e. operating costs, investment costs and Total Annual costs are listed in Table 5.4. It is possible to notice that as we increase the number of periods, we can see an increase in the investment costs and an increase in the TAC. In Table 5.5 is provided more detailed information about the components used to calculate the investment costs. In general, in order to accomplish new operating conditions we have to increase either the areas or the utility consumption, consisting in the tradeoff between the TAC and the flexibility. In the Table 5.6 is listed the problem size and the total CPU time in order to find the solution. In spite of the number of integer variables does not depend on the number of periods, but as we increase the number of periods, the number of real variables and constraints increases.

Table 5.4: Cost data for Example 1 using Formulation 1.

$Periods$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$
1	71409.185	83483.790	154892.974
1,2	82320.915	89280.685	171601.600
1,2,3	86902.826	102896.863	189799.690
1,2,3,4	88871.574	106932.279	195803.853

Table 5.5: Average Utility consumption, number of units and Total Area for Example 1 using Formulation 1.

$Periods$	$Qcu\ (kW)$	$Qhu\ (kW)$	nz	$Area\ Total\ (m^2)$
1	2141.149	491.149	6	336.559
1,2	2316.220	594.720	6	375.205
1,2,3	1824.240	744.240	7	429.312
1,2,3,4	2355.911	669.161	6	492.882

Table 5.6: Problem Dimension and Computational Effort for Example 1 using Formulation 1.

$Periods$	$Single\ Variables$	$Integer\ Variables$	$Single\ Constraints$	$CPU(s)$
1	69	12	77	1.979
1,2	121	12	153	1.718
1,2,3	173	12	229	1.844
1,2,3,4	205	12	305	1.824

The same example was solved using the Formulation 2 proposed by Verheyen and Zhang (2006) and equivalent results are expressed in Table 5.7, 5.8 and 5.9. Comparing the solution with the one obtained with Formulation 1, we can observe a slight reduction in the

TAC, less than 5 %. In terms of CPU time, the computational efforts are equivalent since this is a small problem.

Table 5.7: Cost data for Example 1 using Formulation 2.

$Periods$	$Operating$ $Cost$ $(\$/y)$	$Investment$ $Cost(\$/y)$	$Total\ Annual$ $Cost$ $(\$/y)$
1	71409.185	83483.790	154892.974
1,2	82959.718	87728.920	170688.638
1,2,3	88118.759	97078.585	185197.344
1,2,3,4	85185.614	97864.690	183050.304

Table 5.8: Average Utility consumption, number of units and Total Area for Example 1 using Formulation 2.

$Periods$	Qcu (kW)	Qhu (kW)	nz	$Area$ $Total$ (m^2)
1	2141.149	491.149	6	336.559
1,2	2322.944	601.444	6	364.859
1,2,3	1837.040	757.040	7	390.524
1,2,3,4	2317.112	630.362	7	395.765

Table 5.9: Problem Dimension and Computational Effort for Example 1 using Formulation 2.

$Periods$	$Single$ $Variables$	$Integer$ $Variables$	$Single$ $Constraints$	$CPU(s)$
1	81	12	99	1.721
1,2	133	12	165	1.843
1,2,3	195	12	241	1.848
1,2,3,4	217	12	317	1.941

The decomposition approach based in the Formulation 1 proposed was applied for this example. The main results are presented in Table 5.10. Comparing the computational effort, the application of the decomposition technique is not justified. However, an interesting observation is that the solution obtained was better than the one with no decomposition. Since the problem is not solved to global optimality, only suboptimal solutions were found. Solving the decomposed problem yields a smaller and easier problem to solve, making possible the convergence to better local solutions, which combined provides a postulation of a tighter upper bound. In addition, the second column correspond to the solution obtained after the NLP improvement, where the isothermal mixing assumption is removed and the maximum area is considered by fixing the set of binary variables obtained for solving the Formulation 2, slightly modified for accomplishing no isothermal mixing when split occurs.

Table 5.10: Decomposition Approach for Numerical Example 1.

Periods	*Duality gap*	*# Iterations*	*Total Annual Cost (\$/y)*	*TAC NLP Improv.*	*CPU(s)*
1,2	0	1	167401.768	165909.059	2.92
1,2,3	3.0	2	178212.553	175812.092	8.44
1,2,3,4	3.1	1	187849.489	179630.099	5.90

In Figure 5.5 is depicted the network obtained by SYNHEAT Model considering only nominal conditions. In order to accomplish the periodical changes for the nominal conditions and also for the three critical conditions expressed in Table 5.2, a new configuration depicted in Figure 5.6 is required.

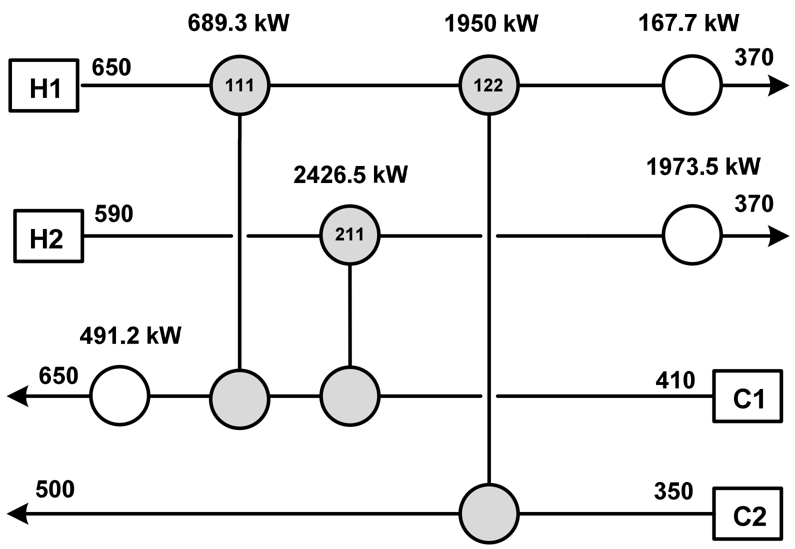

Figure 5.5: Nominal Configuration for Example 1.

5.5.2 Numerical Example 02

The second numerical example involves five hot streams and five cold streams. The nominal data for the problem is listed in Table 5.11. It is assumed expected variations in the inlet temperatures of $\delta_T = 5K$ and a variation of $\delta_F = 10\%$ in the heat capacity flowrates.

The problem was solved using both formulations for the nominal conditions and critical points according to the Table 5.2. The costs for the Formulation 1 and Formulation 2 are listed in Table 5.12 and 5.13 respectively. An interesting observation consists in the fact that using the Formulation 1 was possible to find slightly better solutions, despite the underestimation of the investment costs. The increase of the number of streams, increases the number of nonlinear inequalities in the body of constraints making the Formulation 1 less robust to solve.

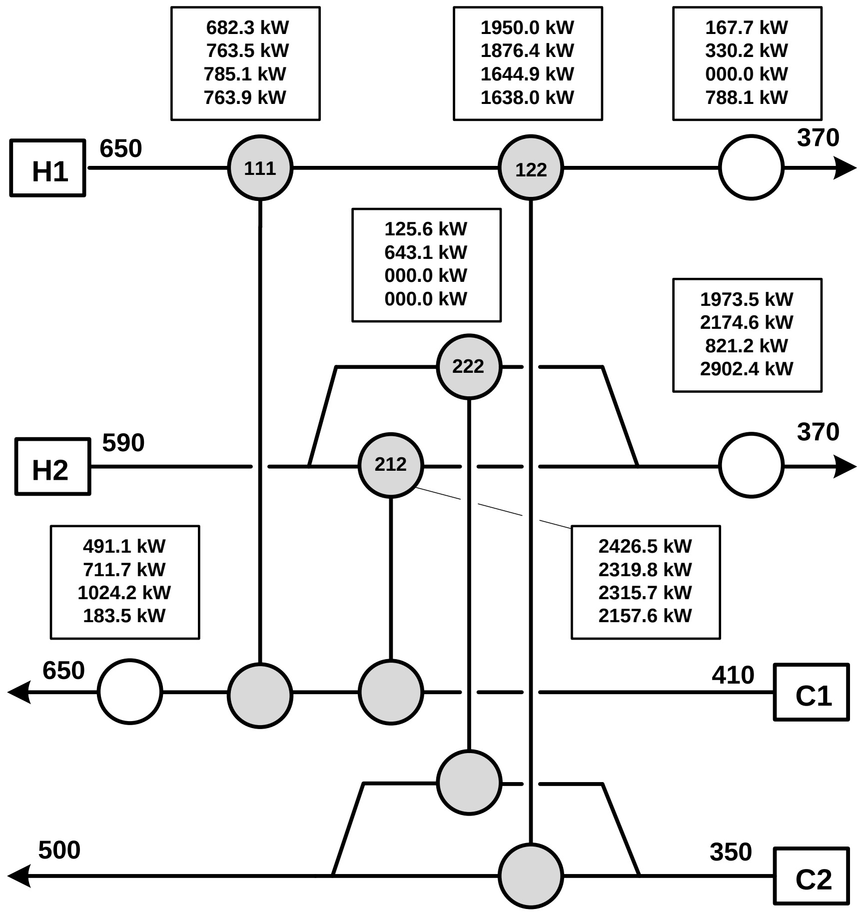

Figure 5.6: Multiperiod synthesis for Example 1 and periods, 1,2,3, and 4..

Table 5.11: Problem data for Example 2.

Stream	T_{in} (ºC)	T_{out} (ºC)	F (kWºC^{-1})	h (kW m^2 ºC^{-1})
H1	320	200	16.67	0.3
H2	480	280	20	0.3
H3	440	150	28	0.3
H4	520	300	23.8	0.3
H5	390	150	33.6	0.3
C1	140	140	14.45	0.3
C2	240	431	16	0.3
C3	100	430	32.76	0.3
C4	180	350	26.35	0.3
C5	200	400	13.9	0.3
CU	100	180		0.3
HU	456	456		0.3

Cost of Heat Exchangers (\$y^{-1}) = 1000+350[Area (m^2)]$^{0.6}$
Cost of Cooling Utility = 11.05 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 5.031 (\$kW^{-1}y^{-1})

Table 5.12: Cost data for Example 2 using Formulation 1.

$Periods$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$	$CPU(s)$
1	45776.918	100353.675	146130.593	2.140
1,2	48065.764	106547.327	154613.091	3.937
1,2,3	39631.910	116694.718	156326.629	5.593
1,2,3,4	46921.341	121468.440	168389.781	4.784

Table 5.13: Cost data for Example 2 using Formulation 2.

$Periods$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$	$CPU(s)$
1	45776.918	100353.675	146130.593	2.140
1,2	48065.764	112796.531	160862.295	4.484
1,2,3	39631.910	117434.097	157066.008	5.905
1,2,3,4	46921.341	122149.127	169070.468	5.231

Table 5.14: Average Utility consumption, number of units and Total Area for Example 2 using Formulation 1.

$Periods$	$Qcu\ (kW)$	$Qhu\ (kW)$	nz	$Area\ Total\ (m^2)$
1	9098.970	0	9	2716.020
1,2	9553.918	0	10	3402.47
1,2,3	7877.541	0	9	3587.066
1,2,3,4	9326.444	0	9	3782.659

Table 5.15: Average Utility consumption, number of units and Total Area for Example 2 using Formulation 2.

$Periods$	$Qcu\ (kW)$	$Qhu\ (kW)$	nz	$Area\ Total\ (m^2)$
1	9098.970	0	9	2716.020
1,2	9553.918	0	9	3071.528
1,2,3	7877.541	0	9	3533.217
1,2,3,4	9326.444	0	9	3731.310

Applying the decomposition approach as possible to obtain better solution, 2.62 % lower for two periods, 7.9 % for three periods and 4.5 % for four periods. Comparing the CPU time, they are almost equivalent.

Table 5.16: Decomposition Approach for Numerical Example 2.

Periods	*Total Annual Cost* ($/y)	*TAC NLP*	*CPU(s)*
1,2	150560.281	148890.207	4.539
1,2,3	143889.615	142311.740	6.265
1,2,3,4	176463.146	175258.181	7.432

The best solution found for the multiperiod operation, the network obtained in Table 5.16 is depicted in Figure 5.7.

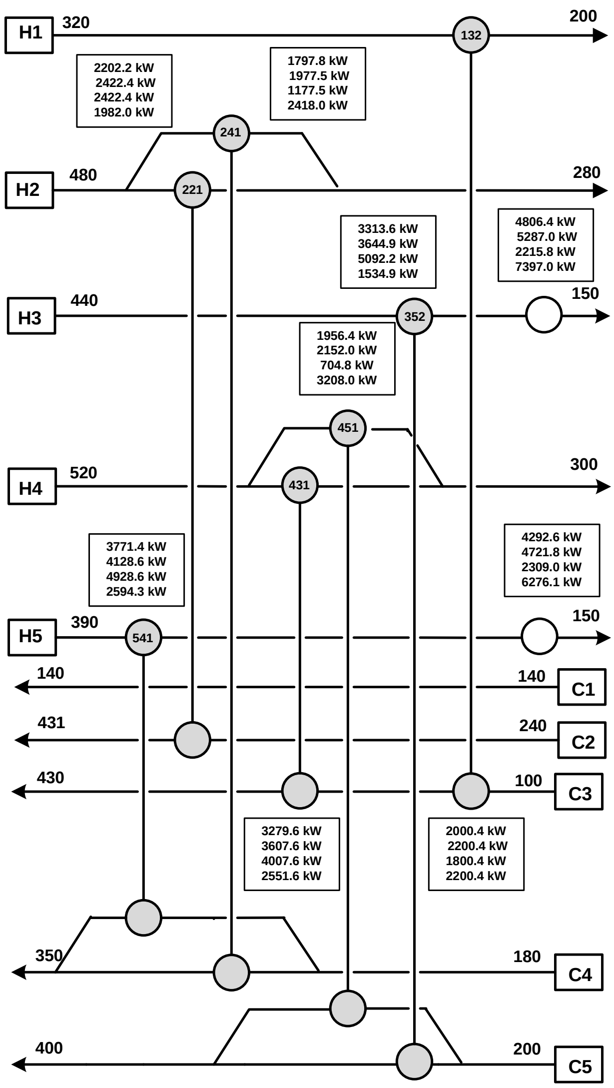

Figure 5.7: Multiperiod Synthesis for periods 1,2,3, and 4 for example 2.

5.5.3 Numerical Example 03

The third numerical example involves eight hot streams and seven cold streams. The nominal and cost data for the problem is presented in Table 5.17. It is assumed expected variations in the inlet temperatures of $\delta_T = 10K$ and a variation of $\delta_F = 5\%$ in the heat capacity flowrates. The minimum number of stages was set to 3.

Tabela 5.17: Problem data for Example 03.

Stream	T_{in} (°C)	T_{out} (°C)	F (kW°C^{-1})	h (kW m^2 °C^{-1})
H1	180	75	30	2
H2	280	120	60	1
H3	180	75	30	2
H4	140	40	30	1
H5	220	120	50	1
H6	180	55	35	2
H7	200	60	30	0.4
H8	120	40	100	0.5
C1	40	230	20	1
C2	100	220	60	1
C3	40	190	35	2
C4	50	190	30	2
C5	50	250	60	2
C6	90	190	50	1
C7	160	250	60	3
CU	25	40		1
HU	325	325		2

Cost of Heat Exchangers (\$y^{-1}) = 8000+500[Area (m^2)]$^{0.75}$
Cost of Cooling Utility / Heating Utility = 10 (\$kW^{-1}y^{-1}) / 80 (\$kW^{-1}y^{-1})

For this problem, only full space solutions using Formulation 1 were generated. The best results are listed in Table 5.18. The problem dimension and the total CPU time spent for each case are listed in Table 5.19.

Table 5.18: Cost data for Example 2 using Formulation 1.

$Periods$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$
1	1180000.00	489885.400	1669885.400
1,2	1099353.853	681779.983	1781133.836
1,2,3	1336188.333	720129.611	2056317.944
1,2,3,4	1591949.949	857970.594	2449920.543

Table 5.19: Problem dimension and computational effort for example 3 using Formulation 1.

Periods	*# Continuous Variables*	*# Integer Variables*	*# Constraints*	*CPU(s)*
1	1047	239	1208	2.077
1,2	1376	239	1541	6.219
1,2,3	1944	239	2666	8.206
1,2,3,4	2512	239	3395	20.171

In Table 5.20 are presented the results for the case were the decomposition approach was applied. For this case it is possible to notice better local solutions and lower computational time. This shows the applicability of the proposed approach. The design obtained for four periods is depicted in Figure 5.8, for simplicity only the nominal conditions are shown.

Table 5.20: Decomposition Approach for Numerical Example 3.

Periods	*Total Annual Cost (\$/y)*	*TAC NLP (\$/y)*	*CPU(s)*
1,2	1720103.588	1713718.930	5.10
1,2,3	1987147.308	1956165.497	8.13
1,2,3,4	2220436.482	2087522.255	10.83

5.6 Conclusions

In this work the multiperiod optimization problem for synthesis of heat exchanger networks was addressed. Different formulations were compared and the block diagonal structure of the problem was exploited. It was proposed a specialized heuristic algorithm that relies on the concept of Lagrangean decomposition. We present an iterative scheme where feasible solutions are postulated from the Lagrangean decomposition subproblems, and the Lagrangean multipliers are updated through a subgradient method. Three numerical examples are used to illustrate the procedure. Despite the high degree of linearity, the model is still nonconvex. Increasing the number of streams and periods, increases the number of nonlinearities. In general, it was possible to find better suboptimal solutions using the proposed scheme even for small scale problems. However the computational efforts is only justified as we increase the problem size. The interesting feature of the proposed method is possible to obtain solutions even whenever is possible to obtain a solution for a given realization of uncertain parameters. The problem solvability is only dependent on the number of streams, and not on the number of scenarios. Furthermore, for medium and large scale problems it is possible to obtain the solutions with lower computational time. Finally, the Lagrangean heuristic decomposition approach can be applied as an alternative procedure to solve multiperiod design of heat exchangers networks.

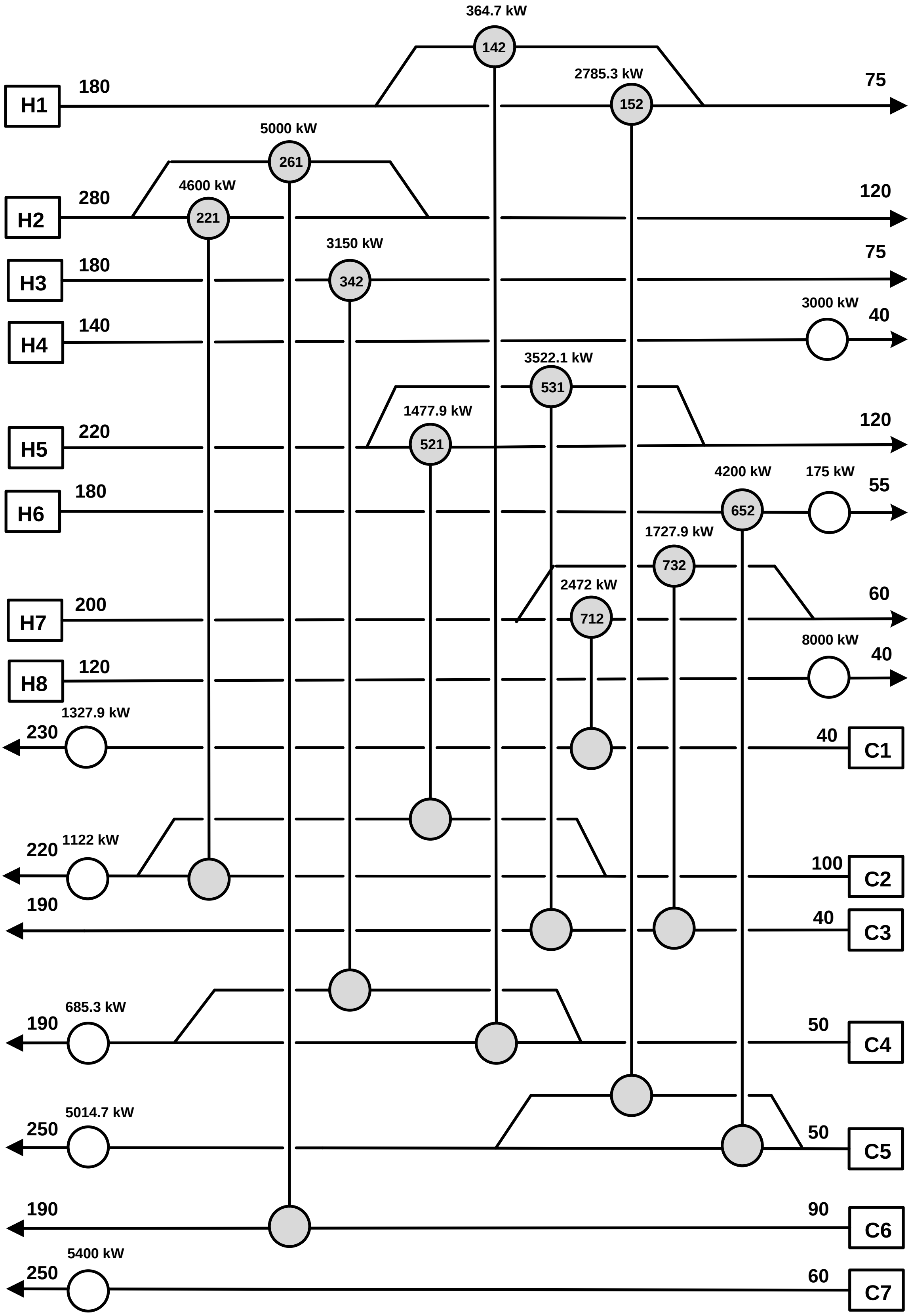

Figure 5.8: Multiperiod Synthesis for periods 1,2,3, and 4 and example 3.

Nomenclature

Abbreviations	
$EMAT$	*exchanger minimum approach temperature*
HEN	*heat exchanger network*
$HENS$	*heat exchanger network synthesis*
$LMTD$	*log mean temperature difference*
TAC	*total annual cost*

Sets	
CP	*set of cold process stream j*
CU	*set of cold utility*
HP	*set of hot process stream i*
HU	*set of hot utility*
P	*set of periods*

Variables	*Units*	
$dt_{i,j,k}$	[°C]	*temperature approach between hot stream i, cold stream j, at location k*
dt_{cui}	[°C]	*temperature approach between hot stream i, and cold utility*
dt_{huj}	[°C]	*temperature approach between cold stream j, and hot utility*
$LMTD_{i,j,k}$	[°C]	*log mean temperature difference between hot stream i, cold stream j, at stage k*
$LMTD_{cui}$	[°C]	*log mean temperature difference between hot stream i, and cold utility*
$LMTD_{huj}$	[°C]	*log mean temperature difference between cold stream j, and hot utility*
Q^{CU}	[kW]	*minimum cold utility requirement*
Q^{HU}	[kW]	*minimum hot utility requirement*
$A_{i,j,k}$	[kW]	*area for heat exchanger between hot stream i and cold stream j at stage k*
$A_{cui,}$	[kW]	*area for heat exchanger between hot stream i and cold utility*
A_{huj}	[kW]	*area for heat exchanger between cold stream j and hot utility*
$q_{i,j,k}$	[kW]	*heat load between hot stream i and cold stream j at stage k*
$q_{cui,}$	[kW]	*heat load between hot stream i and cold utility*
q_{huj}	[kW]	*heat load between cold stream j and hot utility*
q_{ijk}^{p}	[kW]	*heat load between hot stream i and cold stream j at stage k and period p*
q_{cui}^{p}	[kW]	*heat load between hot stream i and cold utility and period p*
q_{huj}^{p}	[kW]	*heat load between cold stream j and hot utility and period p*
t_{i}^{k}	[°C]	*temperature of hot stream i at hot end of stage k*
t_{j}^{k}	[°C]	*temperature of cold stream j at hot end of stage k*
$t_{i,p}^{k}$	[°C]	*temperature of hot stream i at hot end of stage k and period p*
$t_{j,p}^{k}$	[°C]	*temperature of cold stream j at hot end of stage k and period p*

Binary Variables

$z_{i,j,k}$	-	*existence of the match between hot stream i, cold stream j, at stage k*
z_{cui}	-	*existence of the match between hot stream i, and cold utility*
z_{huj}	-	*existence of the match between cold stream j, and hot utility*

Parameters	*Units*	
$\beta_{i,j}$	-	*exponent for the area cost in exchanger i -j*
$c_{i,j}$	-	*cost for heat math between hot stream i and cold stream j*
Ccu_j	[$/kW.yr]	*utility cost coefficient for cooling utility j*
Chu_i	[$/kW.yr]	*utility cost coefficient for heating utility i*
F_i, F_j	[kW/K]	*flow capacity of hot stream i, j*
h_i , h_j	[kW/m^{2}K]	*heat transfer coefficient for hot stream I,j*
T_i^{in}, T_j^{in}	[°C]	*inlet temperature of hot stream i / cold stream j*
T_i^{out}, T_j^{out}	[°C]	*outlet temperature of hot stream i / cold stream j*
δ	[°C]	*expected variation for disturbance range*
U_{ijk}	[kW/K]	*Global heat transfer coefficient*
Ω	[kW]	*upper bound for heat exchangers*
Γ	[°C]	*upper bound for temperature difference*
μ	-	*-Lagrangean multipliers for copy constraints*
λ	-	*Factor for the subgradient method*

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Chapter 6

Simultaneous Synthesis of Flexible Heat Exchanger Networks

Abstract *This work presents a computational framework for automatically generating flexible Heat Exchanger Networks (HEN) over a specified range of expected variations in the inlet temperatures and flowrates of the process streams, such that the Total Annual Cost (TAC) involving the utility consumption, heat exchanger areas and selection of matches are optimized simultaneously. The synthesis of the network was performed using as a basis the superstructure proposed by Yee and Grossmann (1990). The framework SynFlex, which has been implemented in GAMS and MATLAB, is based on a two-stage strategy. The first stage (design phase) is performed prior to the flexibility analysis where the design variables are chosen, i.e. the existence and dimension of the equipments. In the second stage the feasibility of the proposed design is tested so that the control variables are adjusted during operation on the realizations of the uncertain parameters. The proposed computational framework SynFlex yields a HEN design which is guaranteed to operate under varying conditions ensuring stream temperature targets and optimal energy integration. The application of the proposed HEN synthesis strategy and its computational efficiency are illustrated with some numerical examples.*

Extended version of paper presented at European Symposium on Computer Aided Process Engineering (ESCAPE) 21 in Greece, May/June, 2011. This work was also presented at IX Oktoberforum in Porto Alegre-Brazil, October 19-21, 2010.

6.1 Introduction

During the past decades there has been growing awareness both in academia and industry that operability issues need to be considered explicitly at the early stages of process design (Grossmann and Morari, 1984). It is even more important for heat integrated process, since the economic performance of a process is greatly affected by process variations and the ability of the system to satisfy its operational specifications under external disturbances or inherent modeling uncertainty.

Plant flexibility has been recognized to represent one of the important components in the operability of the production process, since it is related to the capability of a process to achieve feasible operation over a given range of uncertain conditions (Grossmann and Floudas, 1987). Uncertainty is an inherent characteristic of any chemical processes. They may have different sources such as: (*i*) unknown disturbances like uncertainty in the process parameters (operating conditions); (*ii*) uncertain model parameters (kinetic parameters, heat transfer coefficients, etc); (*iii*) Discrete uncertainty (failures, equipment availability, etc).

The incorporation of uncertainty in heat exchanger network can be accomplished through a two-stage strategy where a multiperiod optimization problem is coupled iteratively with a flexibility analysis to ensure feasibility over the operational range (see Biegler et al., 1997). In this work, the computational framework SynFlex which implements the two-stage strategy for automatically synthesizing flexible heat exchangers networks, is described.

In the next section, we introduce the problem statement to be addressed in this work. In section 6.3, a deterministic approach for a general process design under uncertainty is presented with corresponding mathematical formulations for design and flexibility analysis. In section 6.4, two numerical examples are presented in order to illustrate the application of SynFlex. Finally, some conclusions and remarks are presented.

6.2 Problem Statement

The problem to be addressed in this paper can be stated as follows. Given are: (*i*) the stream data; (*ii*) a specified range for the uncertainties, i.e. inlet temperatures and heat capacity flowrates, for which the flexibility of the networks is desired (flexibility target); and (*iii*) a minimum temperature approach (ΔT_{min}); The problem consists in synthesizing a heat exchanger network with minimum Total Annual Cost (operating and capital investment cost) that is able to operate feasibly under the specified disturbance range.

6.3 Mathematical Formulation

6.3.1 Background

A general representation of a process design under uncertainty is of the following form:

$$\left.\begin{array}{c} \min\limits_{d,z,x} \underset{\theta\in T}{E}[C(d,x,z,\theta)] \\ s.t.\ h(d,x,z,\theta)=0 \\ g(d,x,z,\theta)\le 0 \\ d\in D, x\in X, z\in Z, \theta\in T \end{array}\right\} \quad (P) \tag{6.1}$$

where d,x, and z are the vectors of design, control and state variables, respectively; θ is the vector of uncertain parameters; $E[C(d,x,z,\theta)]$ is the expected cost function for $\theta \in T = \{\theta|\theta^L \le \theta \le \theta^U\}$; $h(d,x,z,\theta)$ and $g(d,x,z,\theta)$ are the vectors of equality and inequality constraints describing the process model and specifications.

An important question is how systematically determine designs that can accomplish a desired degree of flexibility. In a conventional design optimization problem, the design variables d must be selected so as to minimize the total cost at some nominal values of the uncertain parameters. When the goal of flexibility is also to be accomplished, there are basically two options: Either (i) ensure the flexibility for a fixed parameter range; or (ii) maximize the flexibility measure, while at the same time minimizing cost. The latter problem gives rise to a multi-objective optimization problem, which in fact would normally be solved by optimizing the cost at different fixed values of the flexibility range (Biegler et al., 1997).

Most of the previous works use the termed two stage-strategy. The first stage is prior to the operation (design phase) where the design variables are chosen. At the second stage the control variables z are adjusted during operation on the realizations of $\theta \in T$. It is made the implicit assumption of "perfect control". It means that the control can be immediately adjusted depending on the realization of θ. No delays in the measurements or adjustments in the control are considered.

If the region T is replaced by a discrete set of N points (periods/scenarios), which are somehow specified, the original design problem (P) can be reformulated as a multiperiod optimization problem ($P1$), which is used to deterministically approximate the solution of the optimal design under uncertainty.

$$\left.\begin{array}{c} \min\limits_{d,z,x} \sum_{p=1}^{N} C(d,x^p,z^p,\theta^p) \\ s.t.\ h^p(d,x^p,z^p,\theta^p)=0 \\ g^p(d,x^p,z^p,\theta^p)\le 0 \\ p=1,\dots,N \end{array}\right\} \quad (P1) \tag{6.2}$$

For a fixed design vector d from the solution of $(P1)$ the Flexibility Index problem is solved in order to check whether the design is feasible to operate over the specified range. The uncertainty region is rewritten based on the expected variations along positive $\Delta\theta^+$ and negative directions $\Delta\theta^-$ from nominal conditions θ^N and a positive scalar factor δ, whose maximum value corresponds to the largest scaled hyperrectangle with center in θ^N that can be inscribed within the feasible region.

The two stage strategy is depicted in Figure 6.1. For the selected N periods the multiperiod optimization problem (P1) is solved. The flexibility/feasibility of the multiperiod design must be tested over the space T. If the design is feasible, the procedure terminates; otherwise, the critical point obtained from the flexibility evaluation is included in the current set of θ points, and a new multiperiod formulation is performed. Computational experience has shown that commonly few major iteration must be performed to achieve the feasibility with this method (Biegler et al., 1997).

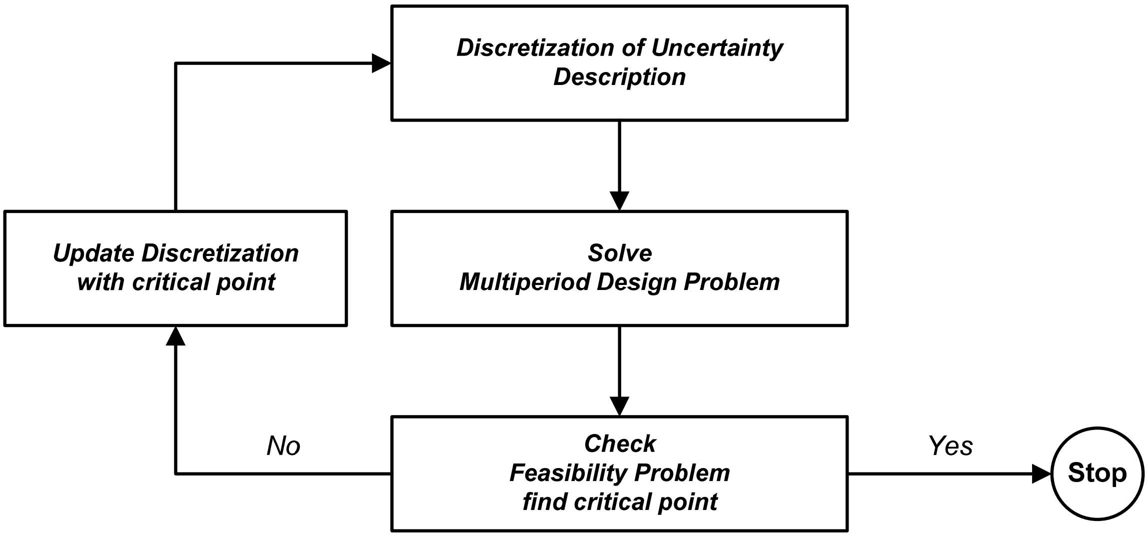

Figure 6.1: Two stage strategy for optimal design under uncertainty.

6.3.2 Mathematical Formulation

Multiperiod Optimization Problem

In this work, the design stage is based on the stage-wise superstructure proposed by Yee and Grossmann (1990). The objective of the model is to find a network that minimizes the total annualized cost, i.e. the investment cost in units and the operating cost in terms of utility consumptions. The superstructure is depicted in Figure 6.2 for the case with two hot streams and two cold streams.

Each hot stream is split into each potential match with all cold streams and vice versa. The outlet flows from the heat exchangers are mixed isothermically, which then defines the stream for the next stage. At the end, utility exchangers are allocated in order to ensure the specifications. The number of stages N_T, is normally set to $max\{N_H, N_C\}$, where N_H and N_C are the number of hot streams and the number of cold streams respectively. The main advantage of this model is that the feasible space of the problem is defined by a set of linear constraints. It generates a model robust to solve.

For the selected N periods the multiperiod optimization problem must be formulated. Different formulations are proposed in the literature. The extension of the SYNHEAT Model for the multiperiod representation is very straightforward. The main issue is that the design variables are invariant over the periods.

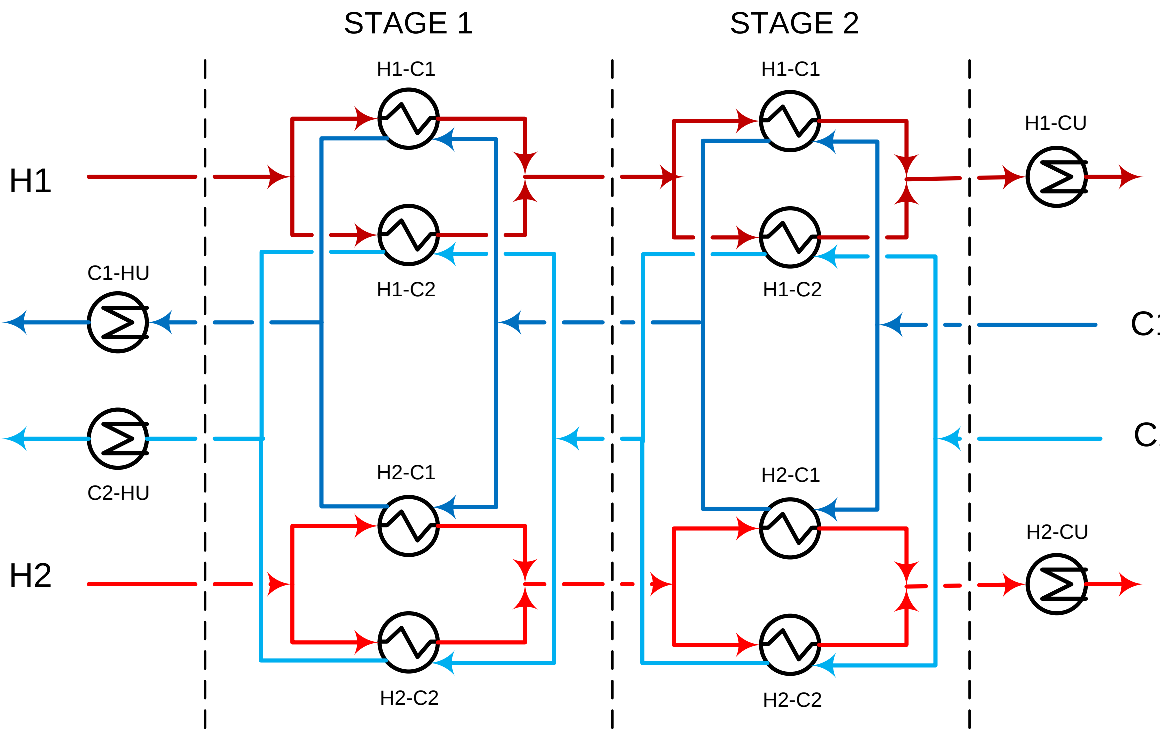

Figure 6.2: Two-stage Superstructure for two hot and two cold streams.

Different multiperiod formulations based on Synheat model are proposed in the literature. In this particular work we consider the formulation proposed by Verheyen and Zhang (2006). This model features the same assumptions of Synheat Model. However some nonlinear inequalities are enforced in order to ensure that the installed area A_{ijk} is the maximum required area A_{ijk}^{p} over all periods p. Due to the direction of the objective function, the constraints $\left(A_{ijk} \geq A_{ijk}^{p}\right)$ are forced to be active for at least the worst case, where the maximum area occurs. This multi-period MINLP model simultaneously minimizes the TAC. The costs included are capital costs for heat exchanger area and unit and the average operating costs for utility consumption. The optimization problem consists of:

$$\min_{x \in \Omega'} \left\{ \begin{array}{c} \sum_{p \in PR} \frac{DOP(p)}{N_P} \left(\sum_{i \epsilon HP} c_{cu} q_{cui}^{p} + \sum_{j \epsilon CP} c_{hu} q_{huj}^{p} \right) + \\ \sum_{i \epsilon HP} \sum_{j \epsilon CP} \sum_{k \epsilon ST} cf_{ijk} z_{ijk} + \sum_{i \epsilon HP} cf_{cu} z_{cui} + \sum_{j \epsilon CP} cf_{hu} z_{huj} + \\ \sum_{p \epsilon PR} \frac{1}{N} \left(\sum_{i \epsilon HP} \sum_{j \epsilon CP} \sum_{k \epsilon ST} c_{ij} \left(A_{ijk}\right)^{\beta} + \sum_{i \epsilon HP} c_{cui} (A_{cui})^{\beta} + \sum_{j \epsilon CP} c_{huj} \left(A_{huj}\right)^{\beta} \right) \end{array} \right\} \quad (6.3)$$

and the feasible space is defined by the following set of constraints:

$$\Omega = \left\{ \begin{array}{c} \left.\begin{array}{c} \left(T_i^{in,p} - T_i^{out}\right)w_i^p = \sum_{\forall k \in ST} \sum_{\forall j \in CP} q_{ijk}^p + q_{cui}^p \\ \left(T_j^{out,p} - T_j^{in,p}\right)w_j^p = \sum_{\forall k \in ST} \sum_{\forall i \in HP} q_{ijk}^p + q_{huj}^p \end{array}\right\} \begin{array}{c} overall \\ heat\ balance \end{array} \\ \left.\begin{array}{c} \left(t_{ik}^p - t_{i,k+1}^p\right)w_i^p = \sum_{\forall j \in CP} q_{ijk}^p \\ \left(t_{jk}^p - t_{j,k+1}^p\right)w_j^p = \sum_{\forall i \in HP} q_{ijk}^p \end{array}\right\} \begin{array}{c} stagewise \\ heat\ balances \end{array} \\ t_{i1}^p = T_i^{in,p}\ ,\ t_{j,N_T+1}^p = T_j^{in,p} \Big\} \begin{array}{c} assignment\ of \\ inlet\ temperature \end{array} \\ \left.\begin{array}{c} t_{ik}^p \geq t_{i,k+1}^p\ ,\ t_{jk}^p \geq t_{j,k+1}^p \\ T_i^{out,p} \leq t_{i,N_T+1}^p\ ,\ T_j^{out,p} \geq t_{j1}^p \end{array}\right\} \begin{array}{c} feasibility\ of \\ temperature \end{array} \\ \left.\begin{array}{c} \left(t_{i,N_T+1}^p - T_i^{out,p}\right)w_i^p = q_{cui}^p \\ \left(T_j^{out,p} - t_{j1}^p\right)w_j = q_{cui}^p \end{array}\right\} utility\ loads \\ \left.\begin{array}{c} q_{ijk}^p - \Lambda_{ij} z_{ijk} \leq 0 \\ q_{cui}^p - \Lambda_i z_{cui} \leq 0 \\ q_{huj}^p - \Lambda_j z_{huj} \leq 0 \end{array}\right\} \begin{array}{c} logical \\ constraints \end{array} \\ \left.\begin{array}{c} dt_{ijk}^p \leq t_{ik}^p - t_{jk}^p + \Gamma_{ij}\left(1 - z_{ijk}\right) \\ dt_{ij,k+1}^p \leq t_{i,k+1}^p - t_{j,k+1}^p + \Gamma_{ij}\left(1 - z_{ijk}\right) \\ dt_{cui}^p \leq t_{i,N_T+1}^p - T_{cu}^{out,p} + \Gamma_i(1 - z_{cui}) \\ dt_{cui}^p \leq T_{hu}^{out,p} - t_{j1}^p + \Gamma_j\left(1 - z_{huj}\right) \end{array}\right\} \begin{array}{c} approach \\ temperatures \end{array} \\ dt_{ijk}^p, dt_{cui}^p, dt_{huj}^p \geq \Delta T_{min} \\ z_{ijk}, z_{cui}, z_{huj} \in \{0,1\} \\ q_{ijk}^p, q_{cui}^p, q_{huj}^p \geq 0 \\ \forall i \in HP, j \in CP, k \in ST, p \in PR \end{array} \right\} \tag{6.4}$$

and the nonlinear inequalities for the area definition:

$$\Omega' = \Omega \cup \left\{ \begin{array}{c} A_{ijk} \geq \dfrac{q_{ijk}^p}{U_{ij} LMTD_{ijk}^p} \\ A_{cui} \geq \dfrac{q_{cui}^p}{U_{cui} LMTD_{cui}^p} \\ A_{huj} \geq \dfrac{q_{huj}^p}{U_{huj} LMTD_{huj}^p} \end{array} \right\} \tag{6.5}$$

The resulting model is a MINLP where the nonlinearities are presented in the objective function and in the block of equations (6.3).

Feasibility Test / Flexibility Index

The design problem can be described by a set of equality constraints I and inequality constraints J, representing the plant operation and design specifications:

$$h_i(d, z, x, \theta) = 0, \quad i \in I \tag{6.6}$$

$$g_j(d, z, x, \theta) \leq 0, \quad j \in J \tag{6.7}$$

where d corresponds to the vector of design variables, z the vector of control variables, x the states variables and θ the vector of uncertain parameters. As has been shown by Swaney and Grossmann (1985), for a specific design, d, given this set of constraints, the design feasibility test problem can be formulated as the max-min-max problem:

$$\chi(d) = \max_{\theta \in T} \min_{z} \max_{\substack{i \in I \\ j \in J}} \begin{Bmatrix} h_i(d, z, x, \theta) = 0 \\ g_j(d, z, x, \theta) \leq 0 \end{Bmatrix} \tag{6.8}$$

where the function $\chi(d)$ represents a feasibility measure for design d. If $\chi(d) \leq 0$, design d is feasible for all $\theta \in T$, whereas if $\chi(d) > 0$, the design cannot operate for at least some values of $\theta \in T$. The above max-min-max problem defines a nondifferentiable global optimization problem, which however can be reformulated as the following two-level optimization problem:

$$\begin{cases} \chi(d) = \max\limits_{\theta \in T} \psi(d, \theta) \\ s.t. \quad \psi(d, \theta) \leq 0 \\ \qquad\quad \psi(d, \theta) = \min\limits_{z} u \\ \qquad\quad s.t. \;\; h_i(d, z, x, \theta) = 0 \\ \qquad\qquad\quad g_j(d, z, x, \theta) \leq u \end{cases} \tag{6.9}$$

where the function $\psi(d, \theta)$ defines the boundary of the feasible region in the space of the uncertain parameters θ. This function regarded as feasibility function projects the space d, z, x, θ in the space d, θ.

Plant feasibility can be quantified by the determining the flexibility index of the design. Following the definition of the flexibility index proposed by Swaney and Grossmann (1985), this metric expresses the largest scaled deviation δ of any expected deviation $\Delta\theta^+$, $\Delta\theta^-$, that the design can handle. The mathematical formulation for the evaluation of design's flexibility is the following:

$$\begin{cases} F = \max \delta \\ s.t. \quad \chi(d) = \max\limits_{\theta \in T} \min\limits_{z} \max\limits_{\substack{i \in I \\ j \in J}} \begin{Bmatrix} h_i(d, z, x, \theta) = 0 \\ g_j(d, z, x, \theta) \leq 0 \end{Bmatrix} \\ \qquad T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\} \end{cases} \tag{6.10}$$

The design flexibility index problem can be reformulated to represent the determination of the largest hyperrectangle that can be inscribed within the feasible region. Following this idea the mathematical formulation of the flexibility problem has the following form:

$$\begin{cases} F = max\,\delta \\ s.t. \quad \psi(d,\theta) = 0 \\ \qquad \psi(d,\theta) = \min_{z} u \\ \qquad s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad\qquad g_j(d,z,x,\theta) \le u \\ \qquad\qquad T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\} \end{cases} \tag{6.11}$$

Vertex Enumeration Method

For the case where the constraints are jointly 1-D quasi-convex in θ and quasi-convex in z it was proven (Swaney and Grossmann, 1985) that the point θ^c that defines the solution to (6.8) lies at one of the vertices of the parameter set *T*. Based on this assumption, the critical uncertain parameter points correspond to the vertices and the feasibility test problem is reformulated in the following manner:

$$\chi(d) = \max_{k \in V} \psi(d,\theta^k) \tag{6.12}$$

where $\psi(d,\theta^k)$ is the evaluation of the function $\psi(d,\theta)$ at the parameter vertex θ^k and V is the index set for the 2^{N_p} vertices for the N_p uncertain parameters θ. In similar fashion for the flexibility index, the problem (6.11) is reformulated in the following way:

$$F = \min_{k \in V} \delta^k \tag{6.13}$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$, $k \in V$, and is determined by the following problem:

$$\begin{cases} \delta^k = \max_{\delta,z} \delta \\ s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) \le 0 \\ \qquad \theta = \theta^N + \delta\Delta\theta^k \\ \qquad \delta \ge 0 \end{cases} \tag{6.14}$$

Based on the above formulations, a direct search method proposed (Halemane and Grossmann, 1983) that explicitly enumerate all the parameters set vertices. To avoid explicit vertex enumeration, two algorithms were proposed by Swaney and Grossmann (1985): (i) a heuristic vertex search and (ii) an implicit enumeration scheme.

Active Set Strategy

The algorithms presented in previous section, rely on the assumption that the critical points correspond to the vertices of the parameter set T which is valid only for the type of constraints assumed above. To circumvent this limitation, a solution approach was proposed based on the following ideas:

(a) Replace the inner optimization problem

$$\begin{cases} \psi(d,\theta) = \min_{z} u \\ s.t. \ \ h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) \leq u \end{cases} \tag{6.15}$$

by the *Karush-Kuhn-Tucker optimality conditions* (KKT):

$$KKT = \begin{cases} \sum_{j\in J} \lambda_j = 1 \\ \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \lambda_j s_j = 0, \ \ j \in J \\ s_j = u - g_j(d,z,x,\theta), \ \ j \in J \\ \lambda_j, s_j \geq 0, \ \ j \in J \end{cases} \tag{6.16}$$

Where s_j are slack variables of constraints j, λ_j, μ_i, are the Lagrange multipliers for inequality and equality constraints, respectively.

(b) For the inner problem the following property holds that if each square submatrix of dimension $(n_z \times n_z)$ where n_z is the number of control variables, of the partial derivatives of the constraints g_j, $\forall j \in J$ with respect to the control variables z is of full rank, then the number of the active constraints is equal to $n_z + 1$;

(c) Utilize the discrete nature of the selection of the active constraints by introducing a set of binary variables y_j to express if the constrain g_j is active. In particular:

$$\begin{cases} \lambda_j - y_j \leq 0, \ \ j \in J \\ s_j - U(1 - y_j) \leq 0, \ \ j \in J \\ \sum_{j\in J} y_j = n_z + 1 \\ \delta \geq 0 \\ y_j = \{0,1\}, \ \ \lambda_j, s_j \geq 0, \ \ j \in J \end{cases} \tag{6.17}$$

Where U represents an upper bound to the slack variables s_j. Note that

For active constraints:

$$y_j = 1 \xrightarrow{yields} \lambda_j \geq 0,\ \ s_j = 0 \tag{6.18}$$

For inactive constraints:

$$y_j = 0 \xrightarrow{yields} \lambda_j = 0,\ \ 0 \leq s_j \geq U \tag{6.19}$$

Based on these ideas, the feasibility test and the flexibility test problem can be reformulated in the following way:

$$Feasibility\ Test:$$

$$P1 \left\{ \begin{array}{l} \chi(d) = max\, u \\ s.t.\ \ h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) + s_j - u = 0 \\ \qquad \sum_{j \in J} \lambda_j = 1 \\ \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \qquad \lambda_j - y_j \leq 0,\ \ j \in J \\ \qquad s_j - U(1 - y_j) \leq 0,\ \ j \in J \\ \qquad \sum_{j \in J} y_j = n_z + 1 \\ \qquad \theta^L \leq \theta \leq \theta^U \\ \qquad \delta \geq 0 \\ \qquad y_j = \{0,1\},\ \ \lambda_j, s_j \geq 0,\ \ j \in J \end{array} \right.$$

$$Flexibility\ Test:$$

$$P2 \left\{ \begin{array}{l} F = min\, \delta \\ s.t.\ \ h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) + s_j - u = 0 \\ \qquad u = 0 \\ \qquad \sum_{j \in J} \lambda_j = 1 \\ \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \qquad \sum_{j \in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i \in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \qquad \lambda_j - y_j \leq 0,\ \ j \in J \\ \qquad s_j - U(1 - y_j) \leq 0,\ \ j \in J \\ \qquad \sum_{j \in J} y_j = n_z + 1 \\ \qquad \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+ \\ \qquad \delta \geq 0 \\ \qquad y_j = \{0,1\},\ \ \lambda_j, s_j \geq 0,\ \ j \in J \end{array} \right.$$

which corresponds to a mixed integer optimization problem either linear or nonlinear depending on the nature of the constraints.

Grossmann and Floudas (1987) proposed the active set strategy for the solution of the above reformulated problems based on the property that for any combination of $n_z + 1$ binary variables that is selected (i.e. for a given set of active constraints), all the other variables can be determined as a function of θ. They proposed a procedure of systematically indentifying the potential candidates for the active set sets based on the signs of the gradients $\nabla_z g_j(d,z,x,\theta)$. The algorithm for the feasibility test problem involves the following steps:

For every potential active set candidate, determine the value $u_k,\ k = 1, \dots, n_{AS}$, through the solution of the following nonlinear programming problem:

$$\begin{cases} u^k = \max u \\ s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) - u = 0, \;\; j \in AS(k) \\ \qquad \theta^L \leq \theta \leq \theta^U \end{cases} \tag{6.20}$$

The solution of the feasibility test is given by:

$$\chi(d) = \max_{k \in AS(k)} u^k \tag{6.21}$$

And for the flexibility index, for each active set candidate,

$$\begin{cases} \delta^k = \max_{\delta,z} \delta \\ s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) - u = 0, \;\; j \in AS(k) \\ \qquad u = 0 \\ \qquad \theta^N + \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+ \\ \qquad \delta \geq 0 \end{cases} \tag{6.22}$$

The solution of the flexibility index problem is given by

$$F = \min_{k \in AS(k)} \delta^k \tag{6.23}$$

Flexibility and Feasibility of HENs

To carry out the flexibility analysis of HENs, all relevant equality and inequality for the HEN model, can be reorganized as described:

$$h(d,z,x,\theta) = \begin{Bmatrix} \sum_{\forall j \in CP} q_{ijk} - (t_{ik} - t_{i,k+1}) w_i \\ \sum_{\forall i \in HP} q_{ijk} - (t_{jk} - t_{jk+1}) w_j \\ q_{cui} - (t_{i,N_T+1} - T_i^{out}) w_i \\ q_{huj} - (T_j^{out} - t_{j1}) w_j \\ T_i^{in} - t_{i1} \\ T_j^{in} - t_{j,N_T+1} \end{Bmatrix} = 0 \tag{6.24}$$

and

$$g(d,z,x,\theta) = \left\{ \begin{array}{c} t_{i,k+1} - t_{ik} \\ t_{j,k+1} - t_{jk} \\ T_i^{out} - t_{i,N_T+1} \\ t_{j1} - T_j^{out} \\ \Delta T_{min} \ + t_{jk} - t_{ik} \\ \Delta T_{min} \ + t_{j,N_T+1} - t_{i,N_T+1} \\ \Delta T_{min} \ + T_{cu}^{out} - t_{i,N_T+1} \\ \Delta T_{min} \ + t_{j1} - T_{hu}^{out} \end{array} \right\} \leq 0 \tag{6.25}$$

Substituting the equations (6.24) and (6.25) in the formulation described in the previous sections it is possible to solve the feasibility and flexibility test. It should be noted that these equations are based on the constraints of Synheat Model, and the overall heat balances are not included because they can be obtained by combining other independent equalities. It ensures the full rank of the partial derivatives of the constraints with respect to the control variables z, which is a premise of the active set strategy. The control variables are chosen as the degrees of freedom during operation, determined by the number of equations minus the number of unknown variables.

6.4 Numerical Examples

6.4.1 Example 1

The problem data and the uncertainty description for this numerical example are presented in Table 6.1. It was assumed only inlet temperatures as uncertain parameters. For this particular case the set of equations (6.24) and (6.25) are linear. Therefore the critical operation conditions are explored on the basis of the vertices of the polyhedral region of uncertainty trough a scalar δ_T (flexibility target). Considering N uncertain parameters, the total number of vertex directions is 2^N, i. e. combinations of the ± directed deviations from the nominal values of the uncertain parameters. Considering the inlet temperatures as uncertain parameters, the total number of vertices V is equal to $2^{(NH+NC)} = 16$.

Table 6.1: Problem data for Ex.1 (Floudas and Grossmann, 1987).

Stream	T_{in} (K)	T_{out} (K)	w (kWK^{-1})	h (kW m^2 K^{-1})
$H1$	583±10	323	1.4	0.16
$H2$	723±10	553	2.0	0.16
$C1$	313±10	393	3.0	0.16
$C2$	388±10	553	2.0	0.16
CU	303	323		0.16
HU	573	573		0.16

Cost of Heat Exchangers (\$y^{-1}) = 5500+4333[Area (m^2)]$^{0.60}$
Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 172.428 (\$kW^{-1}y^{-1})

For the nominal conditions presented in Table 6.1 using the Synheat Model it was generated the Heat Exchanger Network depicted in Figure 6.3. The MINLP model was solved using the solver DICOPT with a CPU time of 0.184 seconds. The resulting configuration has a Total Annual Cost (TAC) of 92.210,14 \$/year and the utility consumption as the minimum possible.

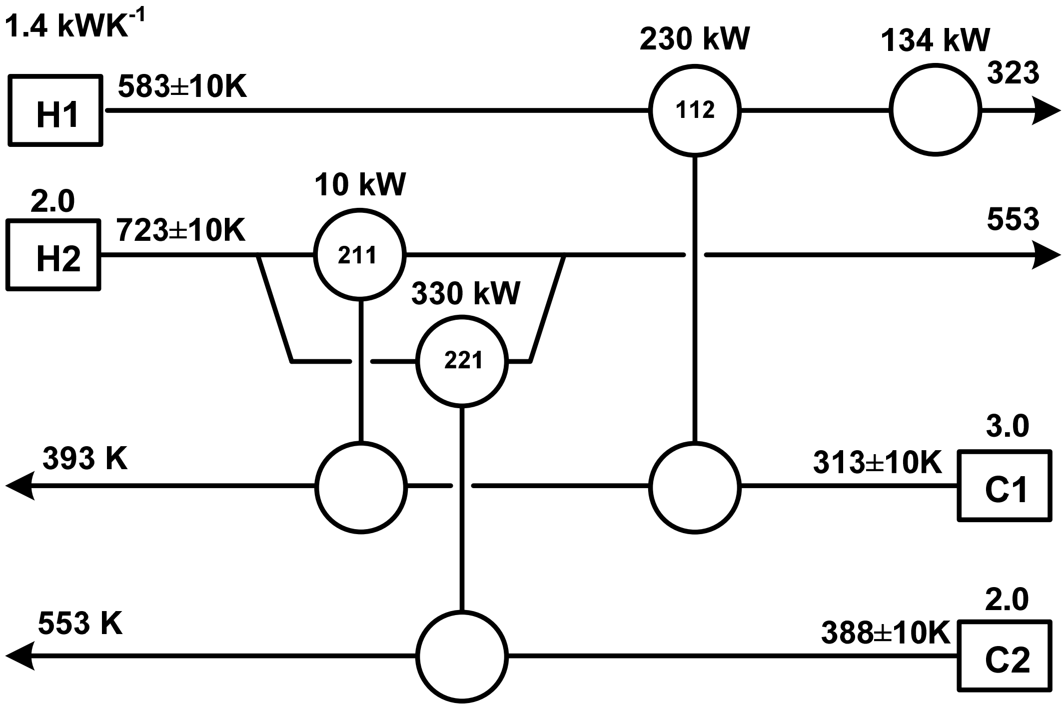

Figure 6.3: Heat Exchanger Network for Example 1.

The inlet temperatures, for each vertex k, and for target flexibility $(\delta_T = 10K)$ are assigned to the inlet temperatures of the HEN configuration through the equations (6.26) and (6.27) as dependent on the vertices of the polyhedral uncertainty region, which is defined by the scalar target flexibility, δ, that acts as a scale factor. The parameters $r_{i,k}$, $r_{j,k}$ are the vertex identifier and take the values of V combinations of the ± directed deviations from the nominal values of the uncertain parameters according illustrated in Table 6.2.

$$T_{i,k}^{in} = T_{i,k}^{in,0} + \delta \Delta T_{i,k}^{in} \quad i \in HP, k = 1, \dots, V \tag{6.26}$$

$$T_{j,k}^{in} = T_{j,k}^{in,0} + \delta \Delta T_{j,k}^{in} \quad j \in CP, k = 1, \dots, V \tag{6.27}$$

where

$$\Delta T_{i,k}^{in} = r_{i,k} \delta_T \quad i \in HP, k = 1, \dots, V \tag{6.28}$$

$$\Delta T_{j,k}^{in} = r_{j,k} \delta_T \quad j \in CP, k = 1, \dots, V \tag{6.29}$$

It was solved 16 LPs subproblems by using CPLEX in order to evaluate the flexibility along each vertex direction. The general results are presented in Table 6.2. The minimum value was identified in the vertices 6, 8, 14, and 16 with the correspondent value of 0.250, which represents the Flexibility Index of the configuration. In other words, for the given design, the configuration can remain feasible only for 25 % of the desired target of 10 K. The total CPU time spent was 0.221 seconds.

Table 6.2: Flexibility Evaluation for each vertex k for Example 1.

$Vertex$ k	$Vertex\ Direction$ $r_{i=1,k}$	$r_{i=2,k}$	$r_{j=1,k}$	$r_{j=2,k}$	$Flexibility\ Index\ Candidate$ δ^k	$CPU(s)$
1	+	+	+	+	3.286	0.013
2	+	+	+	−	7.667	0.011
3	+	+	−	+	15.500	0.012
4	+	−	+	+	7.667	0.012
5	+	+	−	−	7.762	0.012
6	+	−	+	−	**0.250**	0.013
7	+	−	−	+	7.762	0.012
8	+	−	−	−	**0.250**	0.013
9	−	+	+	+	3.286	0.012
10	−	+	+	−	7.667	0.012
11	−	+	−	+	15.500	0.013
12	−	+	−	−	2.823	0.013
13	−	−	+	+	7.667	0.023
14	−	−	+	−	**0.250**	0.011
15	−	−	−	+	2.823	0.027
16	−	−	−	−	**0.250**	0.011

For the structure presented in Figure 6.3 the number of control variables (degrees of freedom) is equal to 0, and hence only one of the 13 constraints described by the equation (20) will be active. It was solved 13 LPs subproblems by using the solver CPLEX in order to evaluate the flexibility considering each inequality as active. The total CPU time was 0.20 seconds, and as expected the same solution was found.

Instead of explicit enumeration of the active set, it is possible to use binary variables to perform this discrete decision. The resulting problem can be solved using one MILP instead of 13 LPs in order to obtain the same result. The general comparison for the Flexibility Index evaluation by these different methods is presented in Table 6.3. It is clear that the MILP formulation for the active set strategy (ASS) had the best computational performance than the vertex enumeration method (VEM).

Table 6.3: General comparison for Flexibility Evaluation by different methods for Ex. 1.

$Method$	$Subproblems$	$Flexibility\ Index\ (FI)$	$CPU(s)$
VEM	16 LPs	0.25	0.221
ASS	13 LPs	0.25	0.200
ASS	1 MILP	0.25	0.054

Once the Flexibility Index is lower than 1, the critical point identified is identified and the current set (only the nominal conditions) is updated with this new point and a second iteration is performed. The new multiperiod is solved and the configuration depicted in Figure 6.4 is found.

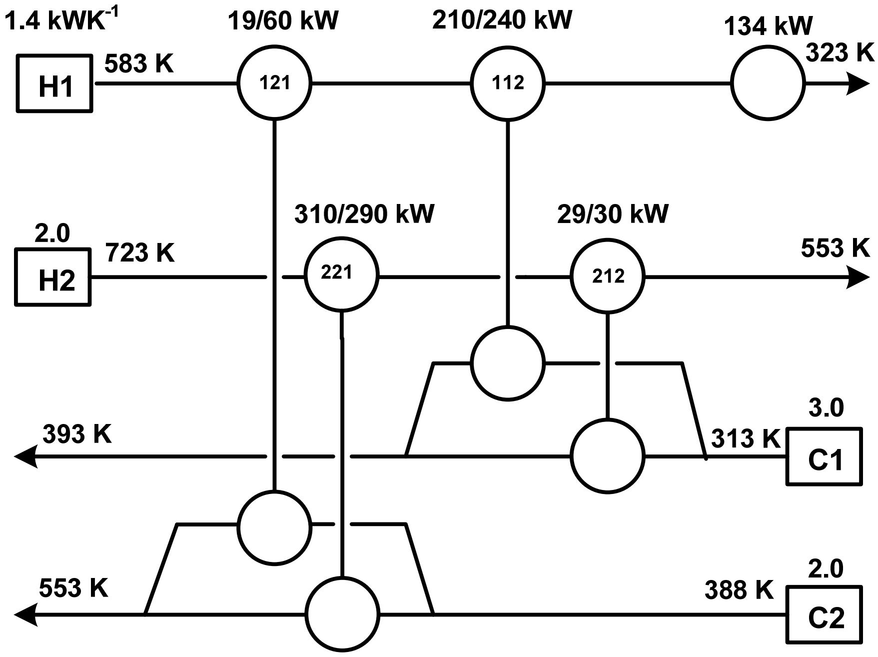

Figure 6.4: Heat Exchanger Network for Example 1 at iteration 2.

The evaluation of the Flexibility Index for the configuration obtained was again solved using the Vertex Enumeration Method (VEM). It was solved 16 LPs subproblems by using CPLEX in order to evaluate the flexibility along each vertex direction. The minimum value was identified in the vertex 16, with the correspondent value of 1.479, which represents the Flexibility Index of the configuration. In Table 6.4 is presented the general comparison for the flexibility index evaluation using active set strategy, where 1 MILP was solved with better computational performance.

Table 6.4: General comparison for Flexibility Evaluation by different methods for Ex. 1.

$Method$	$Subproblems$	$Flexibility\ Index\ (FI)$	$CPU(s)$
VEM	16 LPs	1.479	0.211
ASS	1 MILP	1.479	0.071

The general results are presented in Table 6.5 and the cumulative critical points considered at iteration k is presented in Table 6.6.

Table 6.5: General Results for TSS applied to Example 01.

$Iter.$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$	$Flexibility\ Index$
1	8117	84093	92210	0.250
2	5573	124901	130474	1.429

Once the Flexibility Index is greater than one, the design is sufficient flexible according to the flexibility target, i.e. this configuration is capable to operate feasibly under the expected uncertainty region.

Table 6.6: Points considered for the TSS for Example 01.

$Iter.$	$T_{in}^{H1}(K)$	$T_{in}^{H2}(K)$	$T_{in}^{C1}(K)$	$T_{in}^{C2}(K)$
1	583	723	313	388
2	573	713	303	378

It should be noted that the final configuration supports variations in the inlet temperatures of 14.79 K. The total CPU time for the generation of this flexible design was 0.553 seconds.

6.4.2 Example 2

For the second numerical example it was considered the same nominal conditions as in the example 01. However, three different cases with different uncertainty description were created. The general data for the cases (A,B, and C) are showed in Table 6.7.

For these cases, the uncertainties are presented also in the heat capacity flowrates. The vertex enumeration method cannot be used, since there is no guarantee that the critical point rely on a vertex of the uncertainty region. The equations (6.24) are nonlinear due to the product of temperatures and flowrates generating a set of bilinear constraints that are nonconvex. Using the implicit active set strategy requires the solution of a nonconvex MINLP. Once an important decision is made based on this value, it is very important that this problem be solved to global optimality. The bilinear terms can be replaced by a convex relaxation, e.g. McCormick's envelopes and a spatial branch and bound algorithm can be used to solve this problem. Furthermore, for process synthesis applications, where approximate solutions would be suitable for screening purposes, a quicker way to solve the nonlinear versions of the flexibility index by active set strategy is to linearize the constraint functions around nominal conditions. For example:

$$h(d,z,x,\theta) \cong \quad h(d,z^N,z^N,\theta^N) + \left(\frac{\partial h_i}{\partial \theta}\right)^T (\theta - \theta^N) + \left(\frac{\partial h_i}{\partial z}\right)^T (z - z^N) + + \left(\frac{\partial h_i}{\partial x}\right)^T (x - x^N) \tag{6.30}$$

where (x^N, z^N, θ^N) corresponds to the nominal point. In this way the problem is reduced to a MILP. As discussed by Grossmann and Floudas (1987), these linearizations often yield good approximations.

Table 6.7: Problem data for Ex.2 (Floudas and Grossmann, 1987).

Case	*Stream*	T_{in} (K)	T_{out} (K)	w (kWK^{-1})	h (kW m^2 K^{-1})
A	$H1$	583±10	323	1.4±5%	0.16
	$H2$	723±10	553	2.0±5%	0.16
	$C1$	313±10	393	3.0±5%	0.16
	$C2$	388±10	553	2.0±5%	0.16
	CU	320	323		0.16
	HU	573	573		0.16
B	$H1$	583±10	323	1.4±0.4	0.16
	$H2$	723	553	2.0	0.16
	$C1$	313	393	3.0	0.16
	$C2$	388±5	553	2.0±0.4	0.16
	CU	320	323		0.16
	HU	573	573		0.16
C	HU	573	573		0.16
	$H1$	583	323	1.4±10%	0.16
	$H2$	723	553	2.0±10%	0.16
	$C1$	313	393	3.0±10%	0.16
	$C2$	388	553	2.0±10%	0.16
	CU	320	323		0.16
	HU	573	573		0.16

Cost of Heat Exchangers (\$y^{-1}) = 5500+4333[Area (m^2)]$^{0.60}$
Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 172.428 (\$kW^{-1}y^{-1})

The heat exchanger network for the nominal conditions has already been generated in the previous numerical example and the network obtained can be seen in Figure 6.3. Based on this configuration the flexibility index was evaluated for the three cases using active set strategy. The resulting problem was solved with global optimization (BARON) and by convexification through linearization. The general results are presented in Table 6.8.

Table 6.8: General Comparison for Flexibility Evaluation by different methods for Ex.2.

Case	*Method*	*Subproblems*	*Flexibility Index* (FI)	$CPU(s)$
A	*ASS Linearized*	1 MILP	0.134	0.071
	ASS Global Optimization	1 MNILP	0.136	0.367
B	*ASS Linearized*	1 MILP	0.132	0.069
	ASS Global Optimization	1 MNILP	0.131	0.390

C	*ASS Linearized*	1 MILP	0.149	0.078
	ASS Global Optimization	1 MNILP	0.149	0.410

It is clear that the linearized version equation provides a quite good approximation for the nonlinear model. An important evidence is that the approximate solutions were obtained with much less computational effort.

The two stage strategy was applied for the Case B and the results are summarized in Table 6.9. The procedure converged after 4 iterations for a design with a TAC of 148515 $/ year and a flexibility Index of 1.71.

Table 6.9: Results for TSS applied to Example 02 Case B.

It.	*Operating Cost* ($\$/y$)	*Investment Cost* ($\$/y$)	*Total Annual Cost* ($\$/y$)	*Flexibility Index*	*Flexibility Index* (*lin.*)
1	24758	67452	92210	0.1311	0.1316
2	28823	96083	124905	0.1847	0.2190
3	39540	92563	132194	0.6358	0.6060
4	41749	106765	148515	1.7134	1.9800

This example showed that despite the linearization around nominal conditions generate a problem that can be solved with much less computational effort, it must be applied carefully. For some iterations the linearization provided an error about 20 %. The final configuration obtained is depicted in Figure 6.5.

The total CPU time for the whole procedure was 11.468 seconds for the global optimization and 1.744 for the linearized version. Only a total one second was spent at the design phase (multiperiod problem). In order to speed up the algorithm a good heuristic would be use the linear version and after convergence check using a global optimization technique.

Table 6.10: Results for TSS applied to Example 02 Case B.

Iter.	T_{in}^{H1} (K)	f_{H1} (kW/K)	T_{in}^{C2} (K)	f_{C2} (kW/K)
1	583	1.4	388	2.0
2	593	1.8	383	2.4
3	593	1.8	393	1.6
4	573	1.0	383	2.4

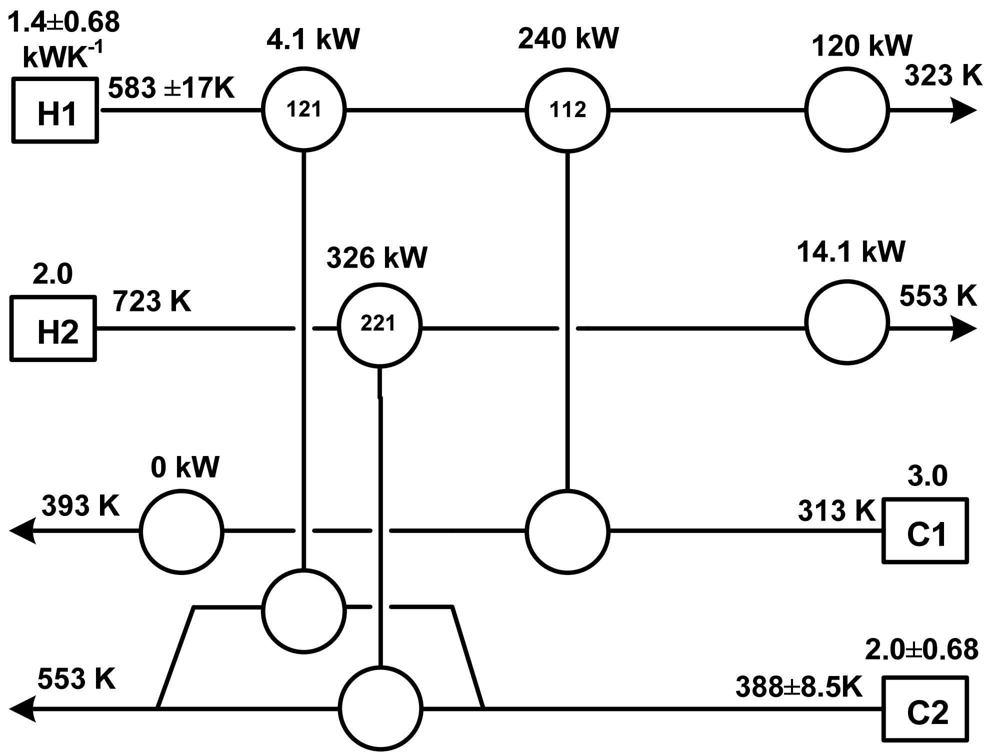

Figure 6.5: Final Configuration for Ex 02.

6.5 General Remarks and Conclusions

It has been developed a computational framework for synthesis of flexible Heat Exchanger Networks; The framework is based on the Two Stage Strategy proposed by Halemane and Grossmann (1983) for design process under uncertainty and oriented to the Synheat Model (Yee and Grossmann, 1991) using Multiperiod Formulations in order to approximate; For the design stage a multiperiod formulation proposed by Verheyen and Zhang (2006); while The Flexibility Analysis is performed using the Active Set Strategy (Grossmann and Floudas, 1987) for the general case. When the uncertain parameters are only in the inlet temperatures the assumption of the critical point relying on a vertex of the uncertainty region is appropriate. We can also use the Active Set Strategy in order to solve for the general case (nonvertex critical point). In that case the problem is nonlinear and a global optimization technique must be used. It is also possible to obtain a good approximation linearizing the problem around the nominal conditions.

In this particular work the main contribution was the integration of different models available in the literature in order to generate an automatic procedure for designing flexible heat exchanger networks. The framework was implemented in GAMS 23.3. Some tricky points during the implementation were overcome, such as, the automatic calculation of the number of degrees of freedom after each design stage and the automatic derivation of the KKT conditions. Despite the numerical examples presented here were in fact small scale problems, the whole procedure was implemented in such way that it can be directly applied for large scale problems. It was developed numerical examples for the flexibility index evaluation to be didactically used in the graduate course Advanced Process System Engineering ministered by Professor Ignacio Grossmann. These routines are available at http://newton.cheme.cmu.edu/interfaces/flexnet/main.html which is an interactive web-based software for Mixed Integer Programming Applications. In this website it is possible to find some available interfaces. It would be also interesting to take a look at the SYNHEAT examples.

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Chapter 7

Simultaneous Synthesis of Flexible and Controllable HENs

***Abstract**: In this work it was developed a computational framework for synthesis of flexible and controllable Heat Exchanger Network. The synthesis of the network was accomplished based on the stage wise superstructure proposed by Yee and Grossmann (1990). It was assumed uncertainty on the inlet temperatures and flowrates. The ability of the design to remain feasible under uncertain conditions, regarded as flexibility, is accomplished based on the termed two stage strategy. A design stage to choose the existence and dimension of the equipments, and an operation stage, for which is checked whether the design selected in the previous step is able to operate over the space of uncertain parameters. If the design is feasible the design is assumed to be flexible; otherwise, the critical point obtained from the flexibility evaluation is included in the current set of periods, and a new multiperiod formulation is solved in order to obtain a new design. Once the flexible design is achieved, a MILP is solved in order to define the control structure selection according to controllability metrics, i.e. the set of manipulated inputs (taken from the general set of potential manipulations) that can ensure the outlet temperatures target using standard feedback controllers, e.g. PI controllers. The effective flexibility is evaluated in order to check if the design is feasible for the given control structure selection, otherwise a new critical point is identified and the multiperiod design is performed again. The application of the proposed HEN synthesis strategy and its computational efficiency are illustrated with some numerical examples.*

Proposed Outlet: Computers and Chemical Engineering.

7.1 Introduction

Heat Exchanger Network Synthesis (HENS) is an important part in the overall chemical process. From the energy point of view we can see an overall process system as three main interactive components (see Figure 7.1), which can be integrated into an operable plant (Aaltola, 2002).

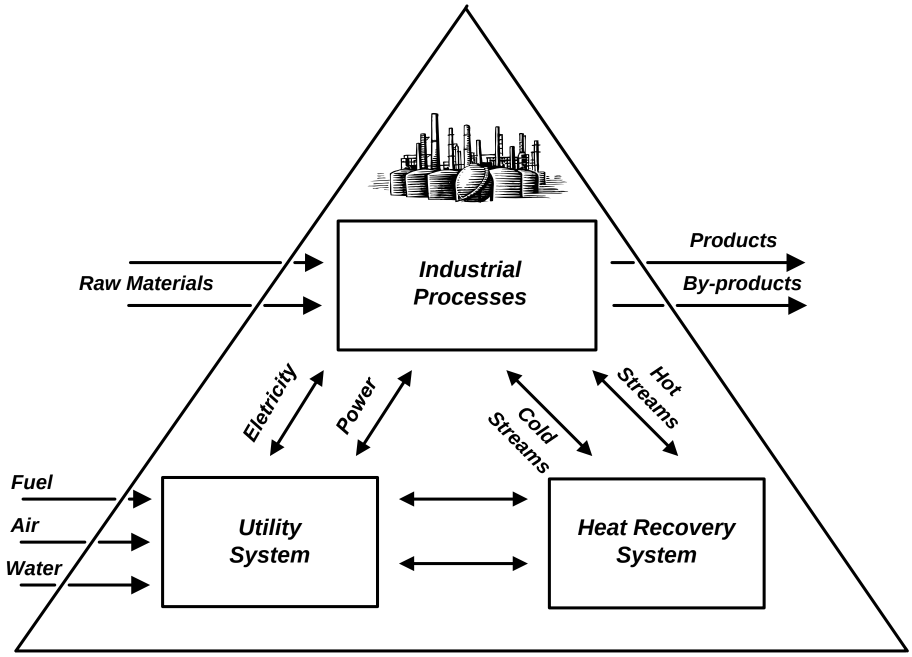


Figure 7.1: An overall process system.

The design of the HEN links the process flowsheet with the utility system and generally involves a large fraction of both the overall plant capital cost, and operating costs in terms of energy requirements being a key factor for a profitable process (Verheyen and Zhang, 2006). The aim of the synthesis consists of finding a network design that minimizes the total annualized cost, i.e. the investment cost in units and the operating cost in terms of utility consumption. The conventional Heat Exchanger Network Synthesis is performed under the assumption of fixed operating parameters at nominal conditions for given specification of a process design. The major techniques are based on sequential (Linnhoff and Hindmarsh, 1983); (Papoulias and Grossmann, 1983; Floudas and Grossmann, 1986) and simultaneous approaches (Ciric and Floudas, 1991); (Yee and Grossmann, 1990). For a recent review see the paper by (Furman and Sahinidis, 2002). The main advantage of simultaneous approaches is that they can handle all the trade-offs properly.

The simultaneous approach of Yee and Grossmann (1990) features interesting characteristics such as being easy to implement and to solve since it is linear constrained making it very attarcttive for extensions. Different extensions have been proposed in the literature: (i) flexibility considerations: Verheyen and Zhang (2006), Chen and Hung (2004) and Konukman, Camurdan, and Akman (2002) (ii) detailed equipment design and fluidaynamic consideration: Serna-González, Ponce-Ortega, and Jiménez-Gutiérrez (2004), Mizutani, Pessoa, Queiroz, Hauan, and Grossmann (2003); (iii) retrofit; (iv) occurrence of phase change (Ponce-Ortega et al., 2008). In this work we are interested in accomplish operability aspects into design, it includes some degree of flexibility and the design of a simple control structure using decentralized and low order controllers once it is the most common strategy in industrial processes making possible the implementation in a practical situation.

Operability considerations, such as flexibility and controllability are very important in a HEN design, but they are usually neglected during the design phase for a given steady state operating point (Glemmstad, 1997). The HEN structure introduces interactions and dramatically change the plant dynamics, and it may make the process more difficult to control and operate (Matinsen, 1994). For a given HEN it is necessary to evaluate its ability to achieve feasible operation over a range of conditions while satisfying performance specifications, regarded as flexibility. It is also important to have a strategy for operating and control which results in reasonable dynamic performance of the plant.

The remainder of the chapter is organized as follows: The section 7.2 provides the problem statement to be adressed in this work, and also the main assumptions. In the section 7.3 is given general ideas about operation and control of HENs while the Section 7.4 presents the outline of the solution strategy. Each problem involved in the proposed method is presented in the following sections. In the section 7.11 three numerical examples are used in order to illustrate the proposed approach, and finally, conclusion and final remarks are drawn in the section 7.12.

7.2 Problem Statement

The problem to be addressed in this paper can be stated as follows. Given are: (*i*) the stream data; (*ii*) a specified range for the uncertainties, i.e. inlet temperatures and heat capacity flowrates, for which the flexibility of the networks is desired (flexibility target); and (*iii*) a minimum temperature approach (ΔT_{min}); The problem consists in synthesizing a heat exchanger network with minimum Total Annual Cost (operating and capital investment cost) that is able to operate feasibly under the specified disturbance range and it is possible to implement using a simple decentralized control system.

This work considers grassroots design cases, and its general multidisciplinary nature involves research in the following areas: (*i*) synthesis of heat exchanger networks; (*ii*) feasibility/flexibility analysis; (*iii*) controllability analysis; (*iv*) optimal operation of heat exchanger networks; (*v*) simultaneous synthesis of flexible heat exchanger networks; (*vi*) optimization based control structure selection; and (*vii*) simultaneous synthesis of flexible and controllable heat exchanger networks.

The following general assumptions are related to this work: (*i*) constant physical properties; (*ii*) non occurrence of phase change; (*iii*) counter-current heat exchanger; (*iv*) shell and tube heat exchangers type; (*v*) neglected pressure drop and further fluid dynamics considerations; (*vi*) non occurrence of fouling; (*vii*) bypasses can be placed across all heat exchangers; (*viii*) utility duties, split fractions and bypasses can be adjusted; (*ix*) perfect control during the flexibility analysis, i.e. control can be adjusted to compensate uncertain parameters (addressed as disturbances) and no delays in the measurements, or adjustments in the control are considered; (*x*) no limitations on flexibility imposed by the control strategy; (*xi*) outlet temperatures as controlled variables; and (*xii*) inlet temperatures and heat capacity flow are addressed as disturbances. Additional considerations are explicitly made afterwards in the text body.

7.3 Design, Operation and Control of HENs

Traditional methods for HENS aim to design a network that yields a reasonable trade-off between capital and operating cost. It is normally assumed that a simple control system can be designed in order to put the network into operation and keep the process operating in the level for which the design was optimized. The control objective in a HEN is usually to maintain the outlet temperatures to specified target values (setpoints, references). In some cases, there may be other control objectives, such the heat duty of the reboiler or condenser in a distillation column that may be integrated in the HEN, or even some internal temperature that has a maximum value, e.g. to prevent decomposition. Furthermore, there may be outlet temperatures without any specified target value (free outlet temperatures). In addition to the regulatory control objective it is important that the utility cost is as small as possible for economic reasons.

For a fixed design a HEN is considered optimal operated if the targets temperatures are satisfied at steady state (main objective); the utility cost is minimized (secondary goal); and the dynamic behaviour is satisfactory (Glemmestad, 1997). During operation, degrees of freedom or manipulated inputs are needed for control and optimization. The different possibilities are shown in Figure 7.2: *1*-Utility Flowrates; *2*-Bypass fraction; *3*-Split fraction; *4*-Process Streams flowrates; *5*-Exchanger area (e.g. flooded condenser); *6*-Recycle (e.g. if exchanger fouling is reduced by increased flowrates).

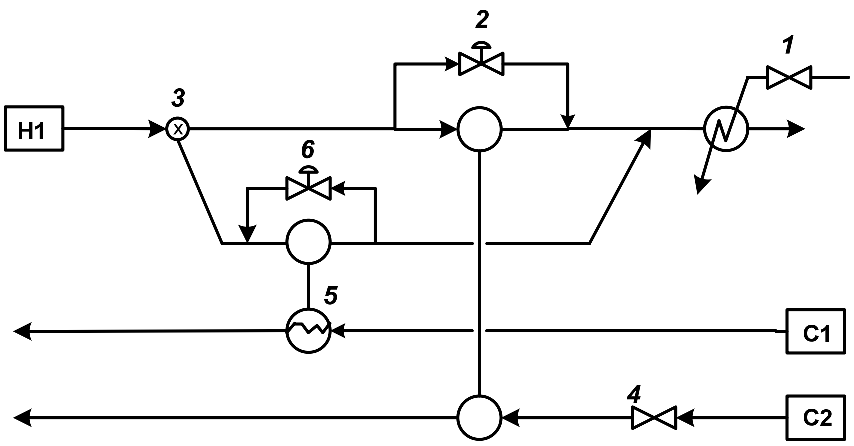


Figure 7.2: Possible manipulated inputs in HENs.

In this work we are interested in general situations, therefore we will consider bypass and in some cases utility flowrates and splitters as manipulated inputs. According to most authors, we assume that the primal control objective is to keep all the outlet temperatures at their targets. For energy optimization the temperatures upstream the utility exchangers are to be as close to the stream target temperatures as possible.

7.4 Proposed Strategy

The incorporation of uncertainty, e.g. disturbances, into design may be possible through a deterministic approach based on the postulation of a finite number of periods (scenarios) to characterize the uncertainty and therefore the problem can be formulated as multiscenario/multiperiod optimization model. The solution of the multiperiod design problem can be embedded in a two stage strategy (see Figure 7.3, and Chapter 6) in order to generate flexible heat exchanger networks (Biegler et al., 1997; Aaltola, 2002; Chen and Hung, 2004 and 2007). Once the design is flexible, the control system strategy can be implemented. Different authors have considered the analysis of controllability and the control system design for HENs in the literature (Matinsen, 1994; Huang and Fan, 2001; Aguilera and Marchetii; 1998; Oliveira, 2001; Lersbarungsuk, 2009). The great majority assume a fixed structure and some units can be added. Depending on the control strategy the full flexibility cannot be achieved. In practice, only with advanced control techniques and/or online optimization it is possible to achieve full flexibility. However it is also interesting whenever is possible to implement a simple control strategy using low order controllers. There are classical methods based on a controllability analysis for designing control strscutures for a given process, which can be embedded in a modified two stage strategy proposed here and depicted in Figure 7.4. For this case the effective flexibility, i.e. the flexibility after the control structure is implemented must be evaluated instead. In the next section each step and its respective mathematical formulation is presented.

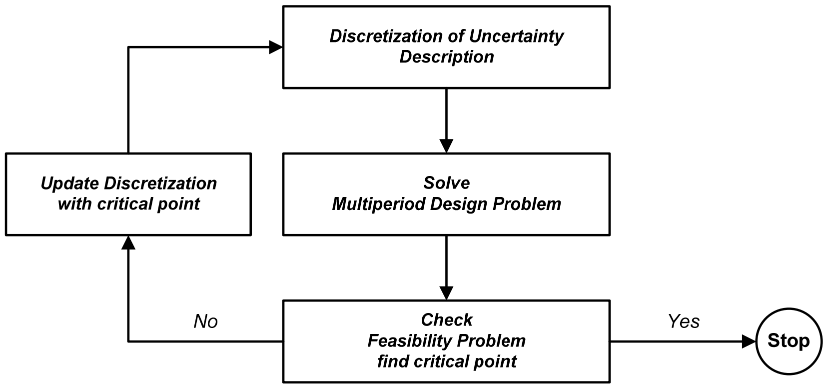


Figure 7.3: Outline of two stage strategy for flexible design.

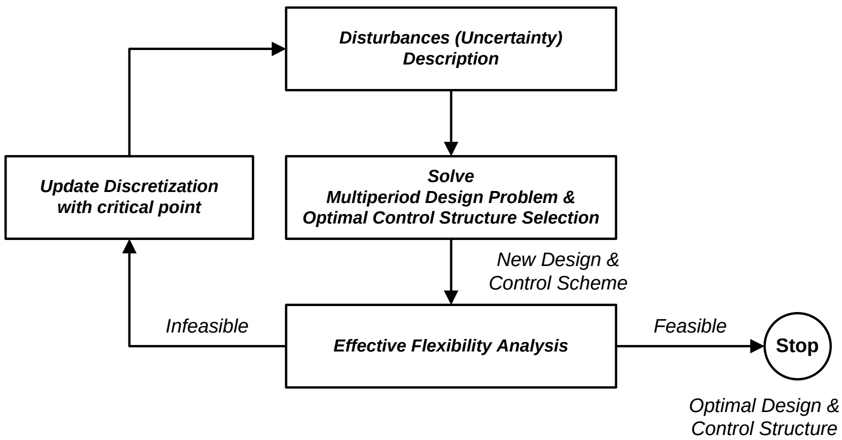


Figure 7.4: Outline of proposed strategy for flexible and controllable design.

7.5 Mathematical Formulation

7.5.1 Multiperiod Synthesis of Heat Exchanger Networks

In this work, the design stage is based on the stage-wise Synheat superstructure proposed by Yee and Grossmann (1990) (see Figure 7.5). The aim of the model is to find a network configuration that minimizes the total annualized cost, i.e. the investment cost in units and the operating cost in terms of utility consumption. Different multiperiod formulations based on SYNHEAT model were proposed in the literature in the last years. In this particular work we consider the formulation proposed by Verheyen and Zhang (2006) and also used by Cheng and Hung (2007). This model features the same assumptions of Synheat Model. However, some nonlinear inequalities are enforced in order to ensure that the installed area is the maximum required area over all periods.

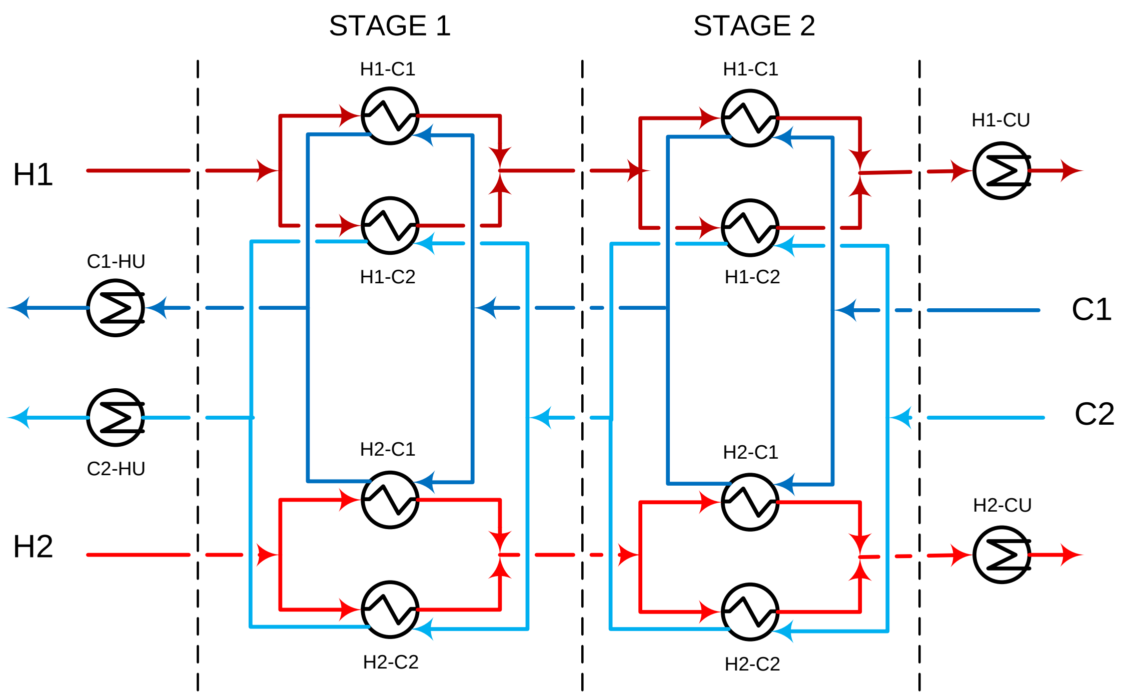


Figure 7.5: Superestructure for Synheat Model (Yee and Grossman, 1990) exemplified for two hot streams, to cold streams and two stages.

In the model formulation, an overall heat balance for each period is needed to ensure sufficient heating or cooling of each process stream:

$$\sum_{k\in ST}\sum_{j\in CP} q_{ijk}^{p} + q_{cui}^{p} = F_i^p\left(T_i^{in,p} - T_i^{out,p}\right), i \in HP, p \in PR \quad (7.1)$$

$$\sum_{k\in ST}\sum_{i\in HP} q_{ijk}^{p} + q_{huj}^{p} = F_j^p\left(T_j^{out,p} - T_j^{in,p}\right), j \in CP, p \in PR \quad (7.2)$$

In order to simplify the model, it is assumed that the outlet streams of each heat exchanger are mixed isothermically at each stage. For that special case, the energy balances around the mixers are no longer needed. For every hot and cold stream the outlet temperatures leaving the heat exchangers at the same stage k are to be the same, and they are associated with the downstream temperature location (t_{ik+1} for hot stream i and t_{jk} for cold stream j). In this way the energy balances for each hot and cold stream around each heat exchanger can be combined into overall heat balances per stage that are linear:

$$\sum_{j \in CP} q_{ijk}^p = F_i^p\left(t_{ik}^p - t_{ik+1}^p\right), i \in HP, k \in ST, p \in PR \tag{7.3}$$

$$\sum_{i \in HP} q_{ijk}^p = F_j^p\left(t_{jk}^p - t_{jk+1}^p\right), j \in CP, k \in ST, p \in PR \tag{7.4}$$

According to the superstructure, the assignment of the inlet temperatures is as follows:

$$t_{i1}^p = T_i^{in,p}, i \in HP, p \in PR \tag{7.5}$$

$$t_{j,NT+1}^p = T_j^{in,p}, j \in CP, p \in PR \tag{7.6}$$

Energy balances for the final utility units define the utility loads for each period:

$$q_{cui}^p = F_i^p\left(t_{i,NT+1}^p - T_i^{out,p}\right), i \in HP, p \in PR \tag{7.7}$$

$$q_{huj}^p = F_j^p\left(T_j^{out,p} - t_{j1}^p\right), j \in CP, p \in PR \tag{7.8}$$

The constraints (7.9) to (7.12) are used to ensure feasibility of temperatures. They specify monotonic decrease in the temperatures along the stages:

$$t_{ik+1}^p \leq t_{ik}^p, i \in HP, k \in ST, p \in PR \tag{7.9}$$

$$t_{jk+1}^p \leq t_{jk}^p, j \in CP, k \in ST, p \in PR \tag{7.10}$$

$$t_{iNT+1}^p \leq T_i^{out,p}, i \in HP, p \in PR \tag{7.11}$$

$$t_{j1}^p \geq T_j^{out,p}, j \in CP, p \in PR \tag{7.12}$$

Upper bound constraints are needed to relate the heat loads q with the binary variables z. In the equations below Ω is an upper bound for the corresponding heat load. If the heat load is not equal to zero the corresponding binary variable is set to one, otherwise the binary variable can be 0 or 1, but the objective function forces the variable to be zero in order to minimize the number of units.

$$q_{ijk}^{p} - \Omega_{ij} z_{ijk} \leq 0, i \in HP, j \in CP, k \in ST, p \in PR \tag{7.13}$$

$$q_{cui}^{p} - \Omega_{i} z_{cui} \leq 0, i \in HP, p \in PR \tag{7.14}$$

$$q_{huj}^{p} \Omega_{j} z_{huj} \leq 0, j \in CP, p \in PR \tag{7.15}$$

In addition, big-M constraints are needed to ensure that the temperature approaches only hold if the heat exchanger exists. The parameter Γ is an upper bound for the temperature difference. If the binary variable is equal to zero the equations are ensured to be feasible. On the other hand, if the binary variable is equal to one, the temperature differences are forced to act as an equality constraint in order to minimize the areas in the objective function.

$$dt_{ijk}^{p} \leq t_{ik} - t_{jk} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST, p \in PR \tag{7.16}$$

$$dt_{ijk+1}^{p} \leq t_{ik+1} - t_{jk+1} + \Gamma_{ij}\left(1 - z_{ijk}\right), i \in HP, j \in CP, k \in ST, p \in PR \tag{7.17}$$

$$dt_{cui}^{p} = t_{i,NT+1} - T_{out}^{CU} + \Gamma_{i}(1 - z_{cui}), i \in HP, p \in PR \tag{7.18}$$

$$dt_{huj}^{p} = T_{out}^{HU} - t_{i1} - T_{out}^{CU} + \Gamma_{j}\left(1 - z_{huj}\right), j \in CP, p \in PR \tag{7.19}$$

The trade-off between investment costs and operating costs are considered by adding the following constraints:

$$dt_{ijk}^{p} \leq \Delta T_{min}, i \in HP, j \in CP, k \in ST, p \in PR \tag{7.20}$$

$$dt_{cui}^{p} \leq \Delta T_{min}, i \in HP, p \in PR \tag{7.21}$$

$$dt_{huj}^{p} \leq \Delta T_{min}, j \in HP, p \in PR \tag{7.22}$$

The next equations are necessary to calculate the area of each unit. The driving forces are calculated by the logarithmic mean temperature difference by Chen approximation for each heat exchanger:

$$LMTD_{ijk}^{p} = \left[dt_{ijk}^{p} dt_{ijk+1}^{p} \frac{dt_{ijk}^{p} + dt_{ijk+1}^{p}}{2}\right]^{1/3} \quad i \in HP, j \in CP, k \in ST, p \in PR \tag{7.23}$$

Similarly for the utility exchangers, the temperature differences are calculated as follows:

$$LMTD_{cui}^{p} = \left[dt_{cui}^{p}\left(T_i^{out} - T_{CU}^{in}\right)\frac{dt_{cui}^{p} + \left(T_i^{out} - T_{CU}^{in}\right)}{2}\right]^{1/3} ,i \in HP, p \in PR \tag{7.24}$$

$$LMTD_{huj}^{p} = \left[dt_{huj}^{p}\left(T_{HU}^{in} - T_j^{out}\right)\frac{dt_{huj}^{p} + \left(T_{HU}^{in} - T_j^{out}\right)}{2}\right]^{1/3} ,j \in CP, p \in PR \tag{7.25}$$

And the area of process-process heat exchangers can be calculated by the following equation:

$$A_{ijk} \geq q_{ijk}^{p}\left(h_i^{-1} + h_j^{-1}\right)/LMTD_{ijk}^{p} \;,i \in HP, j \in CP, k \in ST, p \in PR \tag{7.26}$$

And the areas of the utility units by the following equations:

$$A_{cui} \geq q_{cui}^{p}\left(h_i^{-1} + h_{CU}^{-1}\right)/LMTD_{cui}^{p} \,,i \in HP, p \in PR \tag{7.27}$$

$$A_{huj} \geq q_{huj}\left(h_j^{-1} + h_{HU}^{-1}\right)/LMTD_{huj}^{p} \,,j \in CP, p \in PR \tag{7.28}$$

It is important to notice that due to the direction of the objective function, the constraints (7.26) to (7.28) are forced to be active for at least the worst case, where the maximum area occurs.

Finally, the objective function for the total annual cost (TAC), as a result of the average utility consumption and the invest cost and the complete model are as follows:

$$\begin{aligned} TAC = min \;\; & \frac{1}{N_p}\sum_{p \in PR}\left(c_{CU}\sum_{i \in HP} q_{cui}^{p} + c_{HU}\sum_{j \in CP} q_{huj}^{p}\right) \\ & + c\sum_{i \in HP}\sum_{j \in CP}\sum_{k \in ST} z_{ijk} + c\sum_{i \in HP} z_{cui} + c\sum_{j \in CP} z_{huj} \\ & + \alpha\sum_{i \in HP}\sum_{j \in CP}\sum_{k \in ST} A_{ijk}^{\beta} + \alpha\sum_{i \in HP} A_{cui}^{\beta} + \alpha\sum_{j \in CP} A_{huj}^{\beta} \end{aligned} \tag{7.29}$$

The resulting model consists of the linear equations (7.1) to (7.22), and the nonlinear inequalities (7.26) to (7.28) after substitution of the equations (7.23) to (7.25). The model is a MINLP with nonconvexities only in the equations (7.26) to (7.28) and in the objective function. The areas and the existence of the heat exchanger are invariant for all periods, the heat loads and temperatures are allowed to vary for each period, and the uncertain parameters are selected inside the uncertainty region. Solving this model come up with the network configuration which minimizes the total annual cost.

$$\min_{x\in\Omega}\left\{\begin{array}{c}\sum_{p\in PR}\frac{DOP(p)}{N_P}\left(\sum_{i\epsilon HP} c_{cu}q_{cui}^{p}+\sum_{j\epsilon CP} c_{hu}q_{huj}^{p}\right)+\sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} cz_{ijk}+\sum_{i\epsilon HP} cz_{cui}+\sum_{j\epsilon CP} cz_{huj}\\ \sum_{i\epsilon HP}\sum_{j\epsilon CP}\sum_{k\epsilon ST} c_{ij}\left(A_{ijk}\right)^{\beta}+\sum_{i\epsilon HP} c_{cui}(A_{cui})^{\beta}+\sum_{j\epsilon CP} c_{huj}\left(A_{huj}\right)^{\beta}\end{array}\right\}$$

$$x=\left\{z_{ijk},z_{cui},z_{huj},t_{ik}^{p},t_{jk}^{p};dt_{ijk}^{p},dt_{cui}^{p},dt_{huj}^{p};q_{ijk}^{p},q_{cui}^{p},q_{huj}^{p}i\in HP,j\in CP,k\in ST,p\epsilon PR\right\}$$

$$\left\{\begin{array}{l}A_{ijk}\geq q_{ijk}^{p}\left(h_i^{-1}+h_j^{-1}\right)\Big/\left[dt_{huj}^{p}\left(T_{HU}^{in}-T_j^{out}\right)\frac{dt_{huj}^{p}+\left(T_{HU}^{in}-T_j^{out}\right)}{2}\right]^{1/3}\\ A_{cui}\geq q_{cui}^{p}\left(h_i^{-1}+h_{CU}^{-1}\right)\Big/\left[dt_{cui}^{p}\left(T_i^{out}-T_{CU}^{in}\right)\frac{dt_{cui}^{p}+\left(T_i^{out}-T_{CU}^{in}\right)}{2}\right]^{1/3}\\ A_{huj}\geq q_{huj}\left(h_j^{-1}+h_{HU}^{-1}\right)\Big/\left[dt_{huj}^{p}\left(T_{HU}^{in}-T_j^{out}\right)\frac{dt_{huj}^{p}+\left(T_{HU}^{in}-T_j^{out}\right)}{2}\right]^{1/3}\end{array}\right\}$$

$$\Omega=\left\{\begin{array}{l}\left.\begin{array}{l}\left(T_i^{in,p}-T_i^{out}\right)w_i^{p}=\sum_{\forall k\in ST}\sum_{\forall j\in CP} q_{ijk}^{p}+q_{cui}^{p}\\ \left(T_j^{out,p}-T_j^{in,p}\right)w_j^{p}=\sum_{\forall k\in ST}\sum_{\forall i\in HP} q_{ijk}^{p}+q_{huj}^{p}\end{array}\right\}\textit{overall heat balance}\\ \left.\begin{array}{l}\left(t_{ik}^{p}-t_{i,k+1}^{p}\right)w_i^{p}=\sum_{\forall j\in CP} q_{ijk}^{p}\\ \left(t_{jk}^{p}-t_{j,k+1}^{p}\right)w_j^{p}=\sum_{\forall i\in HP} q_{ijk}^{p}\end{array}\right\}\textit{stagewise heat balances}\\ \left.t_{i1}^{p}=T_i^{in,p},\ t_{j,N_T+1}^{p}=T_j^{in,p}\right\}\textit{assignment of inlet temperature}\\ \left.\begin{array}{l}t_{ik}^{p}\geq t_{i,k+1}^{p},\ t_{jk}^{p}\geq t_{j,k+1}^{p}\\ T_i^{out,p}\leq t_{i,N_T+1}^{p},\ T_j^{out,p}\geq t_{j1}^{p}\end{array}\right\}\textit{feasibility of temperature}\\ \left.\begin{array}{l}\left(t_{i,N_T+1}^{p}-T_i^{out,p}\right)w_i^{p}=q_{cui}^{p}\\ \left(T_j^{out,p}-t_{j1}^{p}\right)w_j=q_{cui}^{p}\end{array}\right\}\textit{utility loads}\\ \left.\begin{array}{l}q_{ijk}^{p}-\Lambda_{ij}z_{ijk}\leq 0\\ q_{cui}^{p}-\Lambda_i z_{cui}\leq 0\\ q_{huj}^{p}-\Lambda_j z_{huj}\leq 0\end{array}\right\}\textit{logical constraints}\\ \left.\begin{array}{l}dt_{ijk}^{p}\leq t_{ik}^{p}-t_{jk}^{p}+\Gamma_{ij}\left(1-z_{ijk}\right)\\ dt_{ij,k+1}^{p}\leq t_{i,k+1}^{p}-t_{j,k+1}^{p}+\Gamma_{ij}\left(1-z_{ijk}\right)\\ dt_{cui}^{p}\leq t_{i,N_T+1}^{p}-T_{cu}^{out,p}+\Gamma_i(1-z_{cui})\\ dt_{cui}^{p}\leq T_{hu}^{out,p}-t_{j1}^{p}+\Gamma_j\left(1-z_{huj}\right)\end{array}\right\}\textit{approach temperatures}\\ dt_{ijk}^{p},dt_{cui}^{p},dt_{huj}^{p}\geq\Delta T_{min}\\ z_{ijk},z_{cui},z_{huj}\in\{0,1\}\\ q_{ijk}^{p},q_{cui}^{p},q_{huj}^{p}\geq 0\\ \forall i\in HP,j\in CP,k\in ST,p\in PR\end{array}\right\}\qquad (P1)$$

7.5.2 Flexibility Index Problem

The design problem can be described by a set of equality constraints I and inequality constraints J, representing the plant operation and design specifications:

$$h_i(d,z,x,\theta) = 0, \quad i \in I \tag{7.30}$$

$$g_j(d,z,x,\theta) \leq 0, \quad j \in J \tag{7.31}$$

where d corresponds to the vector of design variables, z the vector of control variables, x the states variables and θ the vector of uncertain parameters. As has been shown by Swaney and Grossmann (1985), for a specific design, d, given this set of constraints, the design feasibility test problem can be formulated as the max-min-max problem:

$$\chi(d) = \max_{\theta \in T} \min_{z} \max_{\substack{i \in I \\ j \in J}} \begin{Bmatrix} h_i(d,z,x,\theta) = 0 \\ g_j(d,z,x,\theta) \leq 0 \end{Bmatrix} \tag{7.32}$$

where the function $\chi(d)$ represents a feasibility measure for design d. If $\chi(d) \leq 0$, design d is feasible for all $\theta \in T$, whereas if $\chi(d) > 0$, the design cannot operate for at least some values of $\theta \in T$ (see Figure 7.A). The above max-min-max problem defines a nondifferentiable global optimization problem, which however can be reformulated as the following two-level optimization problem:

$$\begin{cases} \chi(d) = \max_{\theta \in T} \psi(d,\theta) \\ s.t. \quad \psi(d,\theta) \leq 0 \\ \qquad\quad \psi(d,\theta) = \min_{z} u \\ \qquad\quad s.t. \;\; h_i(d,z,x,\theta) = 0 \\ \qquad\qquad\quad g_j(d,z,x,\theta) \leq u \end{cases} \tag{7.33}$$

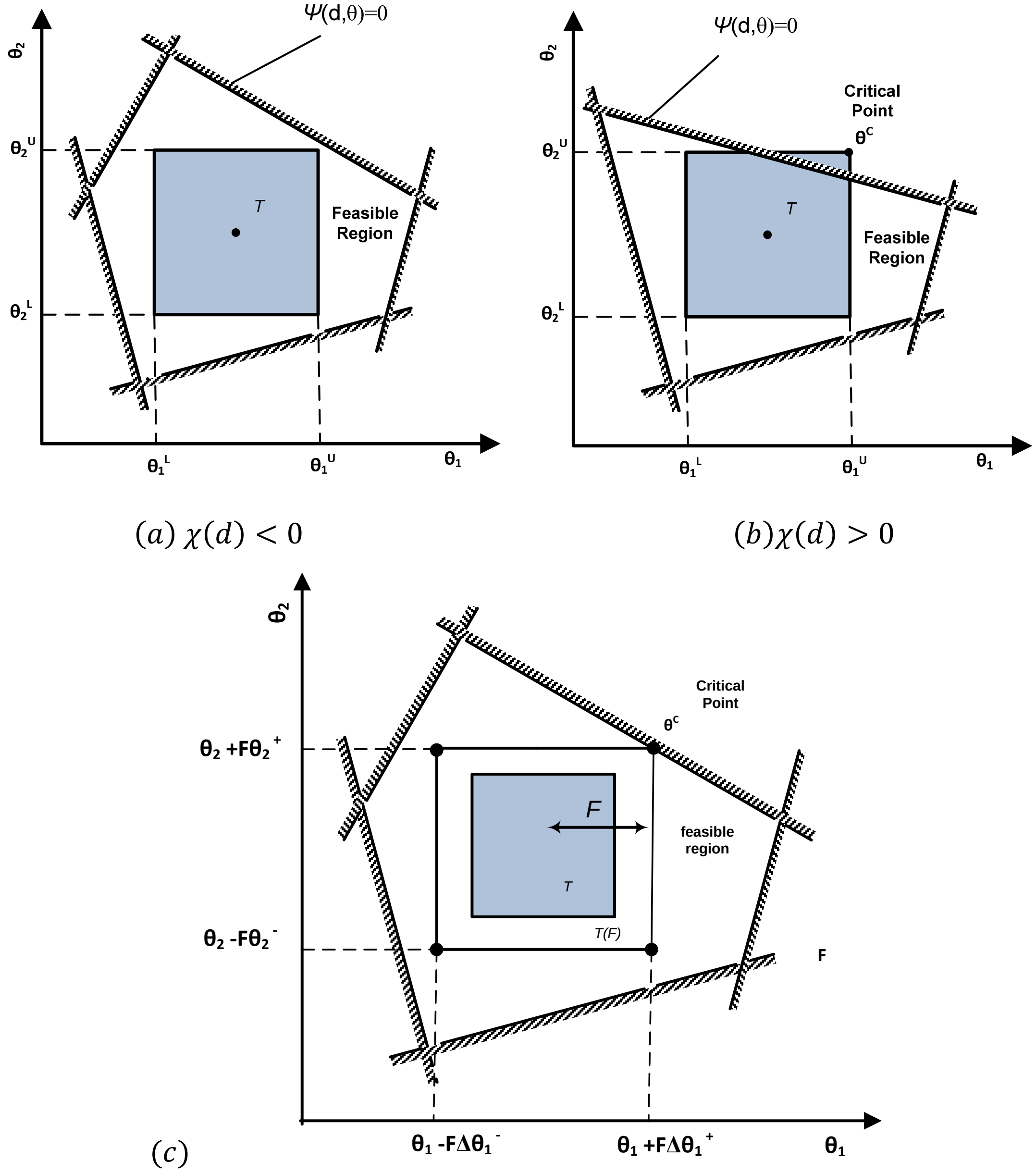
where the function $\psi(d,\theta)$, called as fesibility function, defines the boundary of the feasible region in the space of the uncertain parameters θ. This function projects the space d,z,x,θ in the space d,θ. Its value is negative inside, zero at the boundary and strictly positive outside the feasible region.

Plant feasibility can be quantified by the determining the flexibility index of the design. Following the definition of the flexibility index proposed by Swaney and Grossmann (1985), this metric expresses the largest scaled deviation δ of any expected deviation $\Delta\theta^+$, $\Delta\theta^-$, that the design can handle. The mathematical formulation for the evaluation of design's flexibility is the following:

$$\begin{cases} F = \max \delta \\ s.t. \quad \chi(d) = \max_{\theta \in T} \min_{z} \max_{\substack{i \in I \\ j \in J}} \begin{Bmatrix} h_i(d,z,x,\theta) = 0 \\ g_j(d,z,x,\theta) \leq 0 \end{Bmatrix} \leq 0 \\ \qquad T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \leq \theta \leq \theta^N + \delta\Delta\theta^+\} \end{cases} \tag{7.34}$$

The design flexibility index problem can be reformulated to represent the determination of the largest hyperrectangle that can be inscribed within the feasible region (see Figure 7.A (c)). Following this idea the mathematical formulation of the flexibility problem has the following form:

$$\begin{cases} F = \min \delta \\ s.t. \quad \psi(d,\theta) = 0 \\ \qquad \psi(d,\theta) = \min\limits_{z} u \\ \qquad s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad\qquad g_j(d,z,x,\theta) \le u \\ \qquad\qquad T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\} \end{cases} \tag{7.35}$$



$(a)\ \chi(d) < 0$ $(b)\chi(d) > 0$

(c)

Figure 7.A: Geometric interprtetation of Feasibility Test (a,b) and Flexibility Index (c).

Vertex Enumeration Method

For the case where the constraints are jointly 1-D quasi-convex in t and quasi-convex in z it was proven (Swaney and Grossmann, 1985) that the point θ^c that defines the solution to (7.33) lies at one of the vertices of the parameter set T. Based on this assumption, the critical uncertain parameter points correspond to the vertices and the feasibility test problem is reformulated in the following manner:

$$\chi(d) = \max_{k \in V} \psi(d, \theta^k) \tag{7.36}$$

where $\psi(d, \theta^k)$ is the evaluation of the function $\psi(d, \theta)$ at the parameter vertex θ^k and V is the index set for the 2^{N_p} vertices for the N_p uncertain parameters θ. In similar fashion for the flexibility index, problem (7.35) is reformulated in the following way:

$$F = \min_{k \in V} \delta^k \tag{7.37}$$

where δ^k is the maximum deviation along each vertex direction $\Delta\theta^k$, $k \in V$, and is determined by the following problem:

$$\left\{ \begin{array}{ll} \delta^k = \max\limits_{\delta, z} \delta & \\ s.t. & h_i(d, z, x, \theta) = 0 \\ & g_j(d, z, x, \theta) \leq 0 \\ & \theta = \theta^N + \delta \Delta\theta^k \\ & \delta \geq 0 \end{array} \right. \tag{7.38}$$

Based on the above formulations, a direct search method proposed (Halemane and Grossmann, 1983) that explicitly enumerate all the parameters set vertices. To avoid explicit vertex enumeration, two algorithms were proposed (Swaney and Grossmann, 1985) a heuristic vertex search and an implicit enumeration scheme.

Active Set Strategy

The algorithms presented in previous section, rely on the assumption that the critical points correspond to the vertices of the parameter set T which is valid only for the type of constraints assumed above. To circumvent this limitation, a solution approach was proposed based on the following ideas:

(a) Replace the inner optimization problem

$$\left\{ \begin{array}{l} \psi(d, \theta) = \min\limits_{z} u \\ s.t. \;\; h_i(d, z, x, \theta) = 0 \\ \qquad g_j(d, z, x, \theta) \leq u \end{array} \right. \tag{7.39}$$

by the *Karush-Kuhn-Tucker optimality conditions* (KKT):

$$KKT = \begin{cases} \sum_{j\in J} \lambda_j = 1 \\ \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \lambda_j s_j = 0, \;\; j \in J \\ s_j = u - g_j(d, z, x, \theta), \;\; j \in J \\ \lambda_j, s_j \geq 0, \;\; j \in J \end{cases} \tag{7.40}$$

where s_j are slack variables of constraints j, λ_j, μ_i, are the Lagrangean multipliers for inequality and equality constraints, respectively.

(b) For the inner problem the following property holds that if each square submatrix of dimension $(n_z \times n_z)$ where n_z is the number of control variables, of the partial derivatives of the constraints g_j, $\forall j \in J$ with respect to the control variables z is of full rank, then the number of the active constraints is equal to $n_z + 1$;

(c) Utilize the discrete nature of the selection of the active constraints by introducing a set of binary variables y_j to express if the constrain g_j is active. In particular:

$$\begin{cases} \lambda_j - y_j \leq 0, \;\; j \in J \\ s_j - U(1 - y_j) \leq 0, \;\; j \in J \\ \sum_{j\in J} y_j = n_z + 1 \\ \delta \geq 0 \\ y_j = \{0,1\}, \;\; \lambda_j, s_j \geq 0, \;\; j \in J \end{cases} \tag{7.41}$$

where U represents an upper bound to the slack variables s_j. Note that

For active constraints:

$$y_j = 1 \xrightarrow{yields} \lambda_j \geq 0, \;\; s_j = 0 \tag{7.42}$$

For inactive constraints:

$$y_j = 0 \xrightarrow{yields} \lambda_j = 0, \;\; 0 \leq s_j \geq U \tag{7.43}$$

Based on these ideas, the feasibility test and the flexibility test problem can be reformulated in the following way:

Feasibility Test:

$$(P2')\quad \begin{cases} \chi(d) = max\, u \\ s.t.\quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) + s_j - u = 0 \\ \qquad \sum_{j\in J} \lambda_j = 1 \\ \qquad \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \qquad \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \qquad \lambda_j - y_j \le 0,\ j \in J \\ \qquad s_j - U(1-y_j) \le 0,\ j \in J \\ \qquad \sum_{j\in J} y_j = n_z + 1 \\ \qquad \theta^L \le \theta \le \theta^U \\ \qquad \delta \ge 0 \\ \qquad y_j = \{0,1\},\ \lambda_j, s_j \ge 0,\ j \in J \end{cases}$$

Flexibility Test:

$$(P2)\quad \begin{cases} F = min\, \delta \\ s.t.\quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) + s_j - u = 0 \\ \qquad u = 0 \\ \qquad \sum_{j\in J} \lambda_j = 1 \\ \qquad \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial z} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial z} = 0 \\ \qquad \sum_{j\in J} \lambda_j \frac{\partial g_j}{\partial x} + \sum_{i\in I} \mu_i \frac{\partial h_i}{\partial x} = 0 \\ \qquad \lambda_j - y_j \le 0,\ j \in J \\ \qquad s_j - U(1-y_j) \le 0,\ j \in J \\ \qquad \sum_{j\in J} y_j = n_z + 1 \\ \qquad \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+ \\ \qquad \delta \ge 0 \\ \qquad y_j = \{0,1\},\ \lambda_j, s_j \ge 0,\ j \in J \end{cases}$$

which corresponds to a mixed integer optimization problem either linear or nonlinear depending on the nature of the constraints.

Grossmann and Floudas (1987) proposed the active set strategy for the solution of the above reformulated problems based on the property that for any combination of $n_z + 1$ binary variables that is selected (i.e. for a given set of active constraints), all the other variables can be determined as a function of θ. They proposed a procedure of systematically indentifying the potential candidates for the active set sets based on the signs of the gradients $\nabla_z g_j(d,z,x,\theta)$. The algorithm for the feasibility test problem involves the following steps:

For every potential active set candidate, determine the value u_k, $k = 1,\dots,n_{AS}$, through the solution of the following nonlinear programming problem

$$\begin{cases} u^k = \max u \\ s.t.\quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) - u = 0,\ j \in AS(k) \\ \qquad \theta^L \le \theta \le \theta^U \end{cases} \tag{7.44}$$

The solution of the feasibility test

$$\chi(d) = \max_{k\in AS(k)} u^k \tag{7.45}$$

And for the flexibility index, for each active set candidate

$$\begin{cases} \delta^k = \max_{\delta,z} \delta \\ s.t. \quad h_i(d,z,x,\theta) = 0 \\ \qquad g_j(d,z,x,\theta) - u = 0, \;\; j \in AS(k) \\ \qquad u = 0 \\ \qquad \theta^N + \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+ \\ \qquad \delta \ge 0 \end{cases} \tag{7.46}$$

The solution of the flexibility index problem is given by

$$F = \min_{k \in AS(k)} \delta^k \tag{7.47}$$

Flexibility and Feasibility for HENs

In order to carry out the flexibility analysis of HENs, all relevant equality and inequality for the HEN model, can be reorganized as described:

$$h(d,z,x,\theta) = \begin{Bmatrix} \sum_{\forall j \in CP} q_{ijk} - (t_{ik} - t_{i,k+1})w_i \\ \sum_{\forall i \in HP} q_{ijk} - (t_{jk} - t_{jk+1})w_j \\ q_{cui} - (t_{i,N_T+1} - T_i^{out})w_i \\ q_{huj} - (T_j^{out} - t_{j1})w_j \\ T_i^{in} - t_{i1} \\ T_j^{in} - t_{j,N_T+1} \end{Bmatrix} = 0 \tag{7.48}$$

and

$$g(d,z,x,\theta) = \begin{Bmatrix} t_{i,k+1} - t_{ik} \\ t_{j,k+1} - t_{jk} \\ T_i^{out} - t_{i,N_T+1} \\ t_{j1} - T_j^{out} \\ \Delta T_{min} + t_{jk} - t_{ik} \\ \Delta T_{min} + t_{j,N_T+1} - t_{i,N_T+1} \\ \Delta T_{min} + T_{cu}^{out} - t_{i,N_T+1} \\ \Delta T_{min} + t_{j1} - T_{hu}^{out} \end{Bmatrix} \le 0 \tag{7.49}$$

Substituting the equations (7.48) and (7.49) in the formulation described in the previous sections it is possible to solve the feasibility and flexibility test. It should be noted that these equations are based on the constraints of Synheat Model, and the overall heat balances are not included because they can be obtained by combining other independent equalities. It ensures the full rank of the partial derivatives of the constraints with respect to the control variables z, which is a premise of the active set strategy. The control variables are chosen as the degrees of freedom during operation, determined by the number of equations minus the number of unknown variables.

7.5.3 MILP Formulation for Control Structure Selection

Considering the system described by the following transfer function matrixes:

$$y(s) = G(s)u(s) + G_d(s)d(s) \tag{7.50}$$

where $y(s)$ is the Laplace transform of the ny vector of controlled variables $y(t)$ selected for the base control scheme, $u(s)$ is the Laplace transform of the nu vector of potential manipulated variables $u(t)$, and $d(s)$ is the Laplace transform of the nd vector of disturbances $d(t)$.

MILP Formulation for Calculation of the RGA

The matrix $G(s)$ relates the set of potential manipulated variables $j \in MV = \{1,..,nu\}$ with the controlled variables over the set $i \in CV = \{1,...,ny\}$ where g_{ij} points out the correspondent relation in $G(0)$ with $ny \geq nu$. For any feasible selection of ny manipulated inputs, the matrix $ny \times ny$ $\hat{G}$ that consists of the ny columns of the G matrix that correspond to these inputs, the matrix $\hat{G}$ must be invertible.

If we define the matrix X:

$$X_{ij} = \begin{bmatrix} 1, & \text{if manipulated } j \text{ is used to control controlled variable } i \\ 0, & \text{otherwise} \end{bmatrix} \tag{7.51}$$

The matrix $\tilde{G}$ $ny \times nu$ which includes the columns of the transpose inverse of $\hat{G}$ plus $nu - ny$ zero columns. The elements of this matrix $\tilde{g}_{ij}$ are defined as follows:

$$\sum_{i=1}^{nu} g_{ij}\, \tilde{g}_{\ell j} - \delta_{i\ell} = 0, \qquad \forall\, i, \ell \tag{7.52}$$

where $\delta_{i\ell}$ is the Kronecker delta, and ℓ a set over the controlled variables ($\delta_{i\ell}$ is 1 if $i = \ell$, 0 otherwise). To enforce the fact that the columns for wich the sum $\sum_{i=1}^{ny} X_{ij}$ is zero have to have zero elements, the bounds are added:

$$-\Omega \sum_{i=1}^{ny} X_{ij} \leq \tilde{g}_{\ell j} \leq \Omega \sum_{i=1}^{ny} X_{ij}\,, \qquad \forall\, i, j \tag{7.53}$$

where Ω is a sufficiently large number. The element RGA λ_{ij} can be computed as

$$\lambda_{ij} - g_{ij}\tilde{g}_{ij} = 0, \qquad \forall\, i, j \tag{7.54}$$

In addition, constraints to denote the fact that one and only one manipulated variable has to be assigned to each controlled output:

$$\sum_{i=1}^{ny} X_{ij} - 1 \le 0 \tag{7.55}$$

$$\sum_{j=1}^{nu} X_{ij} - 1 = 0 \tag{7.56}$$

The presented MILP formulation may be used for the effective calculation of the RGA matrix. In the following section, this formulation is used to solve the control structure selection problem.

Minimization of the Interaction (Kookos and Perkins, 2001)

Relative Gain Array (RGA) was introduced by Bristol (1966) and is commonly used as a measure of interaction, an important aspect of integrated process. Input and output should be paired so that the diagonal elements of RGA are close to 1 as possible. Thus, the promising sets of manipulated variables and pairings is based on the minimization of following index:

$$\|RGA - I\|_{sum} = \sum_{i=1}^{ny} \sum_{j=1}^{nu} |\lambda_{ij} - X_{ij}| \tag{7.57}$$

Defining the auxiliary variables $\eta_{ij} = \lambda_{ij} - X_{ij}$ and μ_{ij} as the absolute value of η_{ij} $(-\mu_{ij} \le \eta_{ij} \le \mu_{ij})$. The MILP formulation to find the structure that minimizes the overall interactions can be derived:

$$\left.\begin{array}{l}
min \sum_{i=1}^{ny} \sum_{j=1}^{nu} \mu_{ij} \\
\sum_{i=1}^{ny} X_{ij} - 1 \le 0 \\
\sum_{j=1}^{nu} X_{ij} - 1 = 0 \\
\sum_{i=1}^{nu} g_{ij}\, \tilde{g}_{\ell j} - \delta_{i\ell} = 0, \qquad \forall\, i, \ell \\
\left\{\begin{array}{c}
-\Omega \sum_{i=1}^{ny} X_{ij} \le \tilde{g}_{\ell j} \le \Omega \sum_{i=1}^{ny} X_{ij} \\
\lambda_{ij} - g_{ij}\tilde{g}_{ij} = 0 \\
\eta_{ij} = \lambda_{ij} - X_{ij} \\
-\mu_{ij} \le \eta_{ij} \le \mu_{ij}
\end{array}\right\} \forall\, i, j \\
X_{ij} = \{0,1\}, \quad \mu_{ij} \ge 0 \;\; \forall\, i, j
\end{array}\right\} \text{(S1)}$$

MILP Formulation for Minimization of the Sensitivity to Disturbances

A further objective that can be posed in the control structure selection problem is the disturbance rejection. A measure of the ability of a specific control structure to reject disturbances is the following:

$$\left\|\hat{G}^{-1}G_d\right\|_\infty \tag{7.58}$$

Defining the matrix

$$S = \hat{G}^{-1}G_d \tag{7.59}$$

And also the $nu \times nd$ matrix Σ defined by the equation:

$$\sum_{i=1}^{ny} \tilde{g}_{ij} g_{d,im} - \sigma_{jm} = 0, \qquad \forall\, j, m \tag{7.60}$$

where $m \in DV = \{1, .., nd\}$. The matrix Σ consist of the ny rows of the S matrix that correspond to the inputs selected in the structure as well as $nu - ny$ additional zero rows that correspond to the inputs not selected in the structure. Because of this property, the following equation $\|S\|_\infty = \|\Sigma\|_\infty$ can be stated. The MILP formulation used to find the set of manipulated inputs that is least sensitive to disturbances can be posed:

$$\left.\begin{array}{l}
\min \varphi \\
\displaystyle\sum_{i=1}^{ny} X_{ij} - 1 \le 0 \\
\displaystyle\sum_{j=1}^{nu} X_{ij} - 1 = 0 \\
\displaystyle\sum_{i=1}^{nu} g_{ij}\, \tilde{g}_{\ell j} - \delta_{i\ell} = 0, \qquad \forall\, i, \ell \\
\displaystyle -\Omega \sum_{i=1}^{ny} X_{ij} \le \tilde{g}_{\ell j} \le \Omega \sum_{i=1}^{ny} X_{ij}\, j \\
\displaystyle\sum_{i=1}^{ny} \tilde{g}_{ij} g_{d,im} - \sigma_{jm} = 0, \qquad \forall\, j, m \\
\left\{\begin{array}{c} \displaystyle -\epsilon_j \le \sum_{m=1}^{nd} \sigma_{jm} \le \epsilon_j \\ \epsilon_j - \varphi \le 0 \end{array}\right\} \\
X_{ij} = \{0,1\}, \quad \mu_{ij} \ge 0, \qquad \epsilon_j \ge 0 \;\; \forall\, i, j
\end{array}\right\} \quad (S2)$$

The formulation (*S2*) does not give an answer to the input-output pairing problem but only of a set of manipulated variable. It is due the fact that the disturbance sensitivity measure used does not depend on the pairing but only the sets of controlled and manipulated variables selected. To simultaneously consider the interactions and the disturbance sensitivity the following formulation (*S3*) can be used, where ρ is the weighting coefficient used to assign different contributions of interactions or disturbance sensitivity to the objective function.

Incorporation of Heuristics

In the previous section an MILP formulation for promising control structures was presented. It is very useful the incorporation of qualitative knowledge about the process to eliminate undesirable control structures. Raman and Grossmann (1991) were the first to propose it, presenting a systematic method for converting logical expressions into equivalent mathematical expressions.

The literal P_{ij} is used to represent the logical statement: manipulated variable j is used to control controlled variable i, to this literal is assigned the binary variable X_{ij}. Assuming that specific logical relationships among controlled variables and the potential manipulated variables are expressed in the form of logical propositions, namely, by a set of conjunctions of clauses. The logical propositions are converted into conjunctive normal form (CNF) or disjunctive normal form (DNF). The converted propositions are transformed into linear constraints; see Biegler et al. (1997) for a comprehensive presentation.

$$\left.\begin{array}{l}
min \quad \rho\varphi + (1-\rho)\sum_{i=1}^{ny}\sum_{j=1}^{nu}\mu_{ij} \\
\sum_{i=1}^{ny} X_{ij} - 1 \leq 0 \\
\sum_{j=1}^{nu} X_{ij} - 1 = 0 \\
\sum_{i=1}^{nu} g_{ij}\,\tilde{g}_{\ell j} - \delta_{i\ell} = 0, \qquad \forall\, i,\ell \\
\left\{\begin{array}{c}
-\Omega\sum_{i=1}^{ny} X_{ij} \leq \tilde{g}_{\ell j} \leq \Omega\sum_{i=1}^{ny} X_{ij} \\
\lambda_{ij} - g_{ij}\tilde{g}_{ij} = 0 \\
\eta_{ij} = \lambda_{ij} - X_{ij} \\
-\mu_{ij} \leq \eta_{ij} \leq \mu_{ij}
\end{array}\right\} \forall\, i,j \\
\sum_{i=1}^{ny} \tilde{g}_{ij} g_{d,im} - \sigma_{jm} = 0, \qquad \forall\, j,m \\
\left\{\begin{array}{c}
-\epsilon_j \leq \sum_{m=1}^{nd} \sigma_{jm} \leq \epsilon_j \\
\epsilon_j - \varphi \leq 0
\end{array}\right\} \quad \forall\, j,m \\
X_{ij} = \{0,1\}, \quad \mu_{ij} \geq 0, \qquad \epsilon_j \geq 0 \;\; \forall\, i,j
\end{array}\right\} \quad (S3)$$

7.5.4 Modeling for Disturbance Propagation and Control

Static Modeling

For a given disturbance scenario $\delta T^{in}, \delta w$ and a linearized model can provide an estimation of the static deviation of the system outputs (δT^{out}). The model is embedded into a design procedure for the optimal selection of the control structure, i.e. define the pairs for each control loop. The linear model for a given design (network configuration) is obtained from the model of each unit.

Unit Based Model – A general heat exchanger with bypass on hot and cold side is sketched in Figure 7.6. Based on the mass and energy balances for the heat exchanger, the mixers and splits, the model can be described by the set of equations from (7.61) to (7.65) can generated in a straightforward manner.

The matrices (G_u, G_d^t, G_d^w), are obtained through the linearization of the model HE, using Taylor series expansion, neglecting high-order differentiation terms.

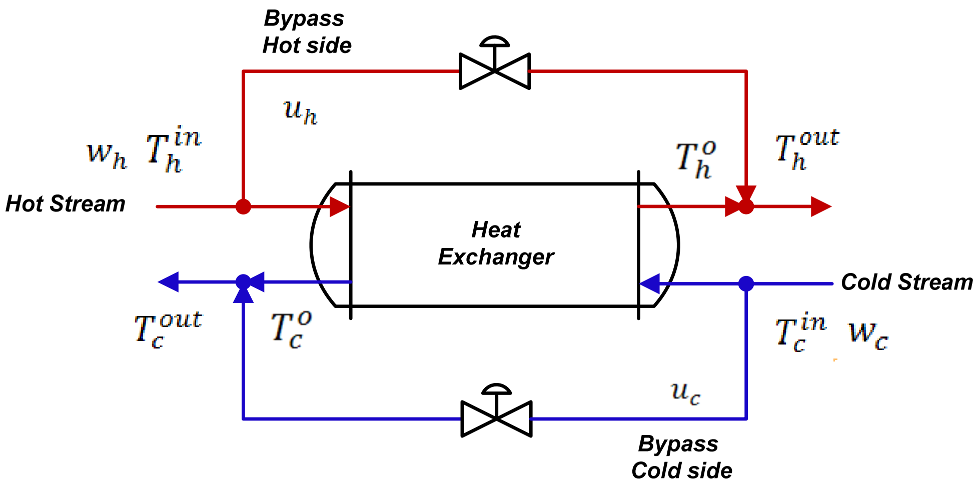


Figure 7.6: General heat exchanger with bypasses.

Unit Model for the system Heat Exchanger with Bypasses.

Mixer Energy Balance:

$$\begin{bmatrix} T_h^{out} \\ T_c^{out} \end{bmatrix} = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{7.61}$$

Inner Heat Exchanger Structure:

$$\begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} = \frac{1}{(R'_h - a')} \begin{bmatrix} R'_h - 1 & 1 - a' \\ R'_h(1-a') & a'(R'_h - 1) \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{7.62}$$

Ratio between effective heat capacity flow rates:

$$R'_h \equiv \frac{(1-u_h)w_h}{(1-u_c)w_c} = \frac{T_c^o - T_c^{in}}{T_h^{in} - T_h^o} \tag{7.63}$$

Ratio between terminal temperature differences:

$$a' \equiv \frac{T_h^{in} - T_c^o}{T_h^o - T_c^{in}} = \exp\left(\frac{U'A}{(1-u_h)w_h}(1-R_h')\right) \tag{7.64}$$

Corrected Global Heat Transfer Coefficient:

$$\frac{1}{U'} = \frac{1}{h_h(1-u_h)^{0.8}} + \frac{1}{h_c(1-u_c)^{0.8}} \tag{7.65}$$

The differentiation of the previous model, composed by equations (7.61) to (7.65), in respect to the inlet temperatures, flowrates and bypass fractions result in the following general model for each heat exchanger:

$$\delta T^{out} = G_{u,E}\delta u + G_{d,E}^{t}\ \delta T^{in} + G_{d,E}^{w}\ \delta w \tag{7.66}$$

HEN Model for Disturbance Propagation and Control

If a HEN contains N_e heat exchangers, a system model can be obtained directly by lumping all unit models for a selected sequence of heat exchanger.

$$\delta T^{*out} = G_{u,E}^{*}\delta u^{*} + G_{d,E}^{*t}\ \delta T^{*in} + G_{d,E}^{*w}\ \delta w^{*} \tag{7.67}$$

The outlet and inlet temperatures flowrates of each heat exchanger is written as a function of the supply and target temperatures and flowrates of the HEN. When the stream is located in between heat exchangers it is called here as intermediate variables.

The temperature vectors δT^{*out} and δT^{*in} can be ordered according to the supply and target temperatures of the streams that are present in the HEN in the following manner.

$$\delta T^{in} = \left[\delta T_{H1}^{s} \dots \delta T_{HN_h}^{s}\ \delta T_{C1}^{s} \dots \delta T_{CN_c}^{s}\ \delta T_1^{m} \dots \delta T_{N_m}^{m}\ \right]^T = [(\delta T^{S})^T(\delta T^{m})^T]^T \tag{7.68}$$

$$\delta T^{out} = \left[\delta T_{H1}^{T} \dots \delta T_{HN_h}^{T}\ \delta T_{C1}^{T} \dots \delta T_{CN_c}^{T}\ \delta T_1^{m} \dots \delta T_{N_m}^{m}\ \right]^T = [(\delta T^{T})^T(\delta T^{m})^T]^T \tag{7.69}$$

The vector δw^* presents N_m redundant heat-capacity flow rates that should be eliminated. This reduces δw^* to δw $[(2N_e - N_m) \times 1]$. Correspondly to

$$G_u^{*} = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} = V_1 G_{u,E}^{*} V_4 \tag{7.70}$$

$$G_d^{*t} = \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} = V_1 G_{d,E}^{*t} V_2 \tag{7.71}$$

$$G_d^{*w} = \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} = V_1 G_{d,E}^{*w} V_3 \tag{7.72}$$

where V_1 to V_4 are the conversion matrices determined by a HEN structure and bypass location. Their derivations are presented in the succeeding section. The reordered model is equivalent to:

$$\begin{bmatrix} \delta T^T \\ \delta T^m \end{bmatrix} = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} \delta u + \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} \begin{bmatrix} \delta T^S \\ \delta T^m \end{bmatrix} + \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} \delta w \tag{7.73}$$

The preceding model (7.73) can be separated into two equations, solving the latter to the intermediate temperatures and substituting in the former yields the following model:

$$\delta T^T = G_{u,hen} \delta u + G_{d,hen}^t \delta T^S + G_{d,hen}^w \delta w \tag{7.74}$$

where

$$G_{u,hen} = G_{u,1} + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{u,2} \tag{7.75}$$

$$G_{d,hen}^t = G_{d,11}^t + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{d,21}^t \tag{7.76}$$

$$G_{d,hen}^w = G_{d,1}^w + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{d,2}^w \tag{7.77}$$

Furthermore, if the vectors of stream temperature and heat capacity flowrates are written based on classification of stream types, the model (7.78) can be written as

$$\begin{bmatrix} \delta T_h^T \\ \delta T_c^T \end{bmatrix} = G_{u,hen} \delta u + \begin{bmatrix} G_{d,hen,h}^t \\ G_{d,hen,c}^t \end{bmatrix}^T \begin{bmatrix} \delta T_h^S \\ \delta T_c^S \end{bmatrix} + \begin{bmatrix} G_{d,hen,h}^w \\ G_{d,hen,c}^w \end{bmatrix}^T \begin{bmatrix} \delta w_h \\ \delta w_c \end{bmatrix} \tag{7.78}$$

Network Structural Representation – As stated in the proceeding section, the transformation matrices V_1 through V_4 are structure dependent. According to the sequence of equipment considered, the original vector of output temperatures (δT^{*out}) will present a defined order involving the target temperatures (δT^T) and the intermediate temperatures (δT^m).

Derivation of V_1. Each element of matrix V_1 has a value 0 or 1 relating the original vector δT^{*out} with the ordered vector δT^{out}. First, the matrix V_1 must have all elements set to 0. The first row of $V_1(i)$ that corresponds to the $\delta T_{h_1}^T$ relation, considering that this target is located in the k position in the disordered vector, set $V_1(i,k)$=1. It should be noted that in case of stream split, where the same temperature enters two or more heat exchangers, there will be more than one position that represent the same target. Then, in a more general way k consist in a vector of corresponding positions. The procedure must be repeated until the last row of δT^{out}.

Derivation of V_2. The matrix V_2 is generated analogously to the matrix V_1. Each element of V_2 has a value 0 or 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to $\delta T^S_{h_1}$ relation, select the k positions that this input appears in the vector δT^{*in} and for each position, set $V_2(k, j)$=1. Repeat the procedure until the last column.

Derivation of V_3. Each element of V_3 has a value between 0 and 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to δw_{h_1}relation, select the k positions that this input appears in the vector δw^* and for each position, substitute by the split fraction of the original stream flowrate, $V_3(k, j) = x_s$. Repeat the procedure until the last column.

Derivation of V_4.. Each element of V_4 has a value 0 or 1. This matrix is determined by the bypass selection in a HEN, i.e. $\delta u = V_4 \delta u_{sel.}$. If is desirable a model with all possible candidates, this matrix must be an identity matrix. In order to derive V_4, first all elements must be set to zero. Select the first column (j) that corresponds the first selected manipulated input $\delta u_{sel.}(1)$, select the k position that this input appears in the vector δu, set $V_4(k, j) = 1$. Repeat the procedure until the last column.

Dynamic Model for Disturbance Propagation and Control

In this work it is considered a lumped compartment or “multicell” model of a heat exchanger is depicted in Figure 7.7. The model is based on the hypothesis that a heat exchanger dynamic behavior can be described by a series of N ideal mixing tank. In addition to ideal mixing tank assumptions, it is assumed: (*i*) constant densities; (*ii*) constant specific heat capacities; (*iii*) constant and flow independent heat transfer coefficient; (*iv*) no phase changes; (*v*) pressure drop neglected; and that exchanger area A and volume V are equally distributed over the N cells.

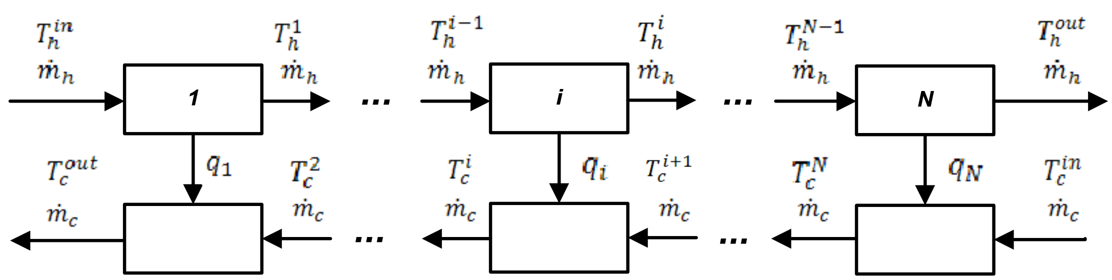


Figure 7.7: Sketch of mixing tank model.

The model for each stage can be described by the following equations:

$$\rho_h V_h^i Cp_h \frac{dT_h^i}{dt} = \dot{m}_h Cp_h \left(T_h^{i-1} - T_h^i\right) - UA^i \Delta T_{ef}^i \tag{7.79}$$

$$\rho_c V_c^i Cp_c \frac{dT_c^i}{dt} = \dot{m}_c Cp_c \left(T_c^{i+1} - T_c^i\right) + UA^i \Delta T_{ef}^i \tag{7.80}$$

The heat transfer area of each cell ($A^i = A/N$) is determined by the total area (A) and the number of tanks (N). The volume of hot and cold fluid in each cell is determined by the total volume in the tube side and the hot side and the total number of cells. Supposing the hot fluid flowing through the shell and the cold fluid flowing through the tubes, we have:

$$V_h^i = \frac{V_h}{N} = \frac{\pi N_t L (D_t - 2\delta_t)^2}{4N} \tag{7.81}$$

$$V_c^i = \frac{V_c}{N} = \frac{\pi D_s^2 L - \pi N_t L D_t^2}{4N} \tag{7.82}$$

The effective temperature driving force for each cell can be represented using different alternatives. The first alternative underestimates the transferred heat at steady-state since the driving forces are less than for ideal countercurrent flow, the arithmetic mean compensates for the underestimation and the logarithmic mean give perfect accordance at steady-state. However this alternative may give serious problem in a dynamic simulation, because it is not defined when the temperature differences are equal, and for example, in a dynamic simulation for an inlet temperature can result in crossover in the heat exchanger until steady-state be reached. The Patterson approximation (Patterson, 1984) and Chen approximation (Chen, 1987) are good approximations of LMTD and can be used to avoid discontinuity when the temperature differences are equal but both give the same problems as LMTD when crossover occurs, since they involve geometric mean, thus they are not suited for dynamic simulations.

Pure Mixing Tank Model:

$$\Delta T_{ef}^i = T_h^i - T_c^i \tag{7.83}$$

Arithmetic mean Temperature difference (AMTD):

$$\Delta T_{ef}^i = \frac{\left(T_h^{i-1} - T_c^i\right) + \left(T_h^i - T_c^{i+1}\right)}{2} \tag{7.84}$$

In addition, the dynamic model for the utility units can be described as follows:

$$\rho_h V_h Cp_h \frac{dT_{hi}^{out}}{dt} = \dot{m}_h Cp_h \left(T_{hi}^{out,0} - T_{hi}^{out}\right) - q_{cui} \tag{7.85}$$

$$\rho_c V_c Cp_c \frac{dT_{cj}^{out}}{dt} = \dot{m}_c Cp_c \left(T_{cj}^{out,0} - T_{cj}^{out}\right) + q_{huj} \tag{7.86}$$

7.5.5 Effective Flexibility Index

In the subsection 7.5.2 it was assumed that all degrees of freedom can be adjusted during the operation. However, it is important to be aware that the actual flexibility may be limited by the control strategy. Even if the HEN is sufficiently flexible, there is no guarantee that the control strategy will adjust the manipulations such that full flexibility is maintained. Therefore, the effective flexibility here is defined as the ability of a controlled HEN to maintain feasible steady state operation for the given uncertainty range. In such way, the effective flexibility is not only a property of the structure by itself as the flexibility but it also depends on the control strategy. It is also important to note that the flexibility is an upper bound for the effective flexibility, and they are equivalent if the number of control variables nz is equal to zero. It means that there is no extra degree of freedom since all of them were consumed by the control strategy.

In order to compute the effective flexibility some minor modifications in the original strategy are necessary. Each heat exchanger contributes with one possible manipulation, i.e. bypass on hot or cold side. We can separate the process to process heat exchanger in two groups: (*i*) if it was selected to be bypassed; (*ii*) or if it is not. The second group corresponds to the subset of heat exchangers from which we can not adjust the bypass across them during the operation. However, the heat load of this heat exchanger will still vary, but not freely, but according to the expression (7.88). The expression consists of the upper bound limited by thermal efficiency. Aguilera and Marchetti (1998) focused that if stream splits are not used as manipulations and only single bypasses are used in HENs, then the optimal operation of HENs can be formulated as a linear problem.

$$q_{ijk}^{p} \leq P_{h,ijk} w_i \left(t_{ik}^{p} - t_{j,k+1}^{p}\right) \text{, for } HE \in CS \tag{7.87}$$

$$q_{ijk}^{p} = P_{h,ijk} w_i \left(t_{ik}^{p} - t_{j,k+1}^{p}\right) \text{, for } HE \in CS \tag{7.88}$$

were

$$P_{h,ijk} = \frac{NTU_{h,ijk}\left(1 - e^{NTU_{c,ijk} - NTU_{h,ijk}}\right)}{NTU_{h,ijk} - NTU_{c,ijk} e^{NTU_{c,ijk} - NTU_{h,ijk}}} \tag{7.89}$$

$$NTU_{h,ijk} = \frac{UA^{max}}{w_i}, NTU_{c,ijk} = \frac{UA^{max}}{w_j} \tag{7.90}$$

7.5.6 Outline of the solution strategy

The outline of the solution strategy is depicted in Figure 7.8. The procedure starts with the design for nominal conditions, solving the the problem P1. And the problem P2 is solved in order to evaluate the Flexibility index for the given design. If the design is not flexible, i.e. the flexibility index is not greater than one; the critical point that defines the solution of P2 is added to the nominal conditions and the problem P1 is solved again. Otherwise it is generated the static model for the design and the MILP for the control structure selection is solved. This problem may have multiple solutions, in order to come up with all possible solutions integer cuts are added cumulatively in order to prevent the same solution to come out again until there is a change in the objective function. For each control structure we can evaluate the effective flexibility index to find the structures that could be implemented to reject the disturbance level.

Once we have found the best design, with minimum *TAC*, able to remain feasible under uncertain conditions, and able to operate with the given control structure it is possible to generate the dynamic model and the transfer function model and design low order controllers, and then dynamic performance of the closed loop can be checked.

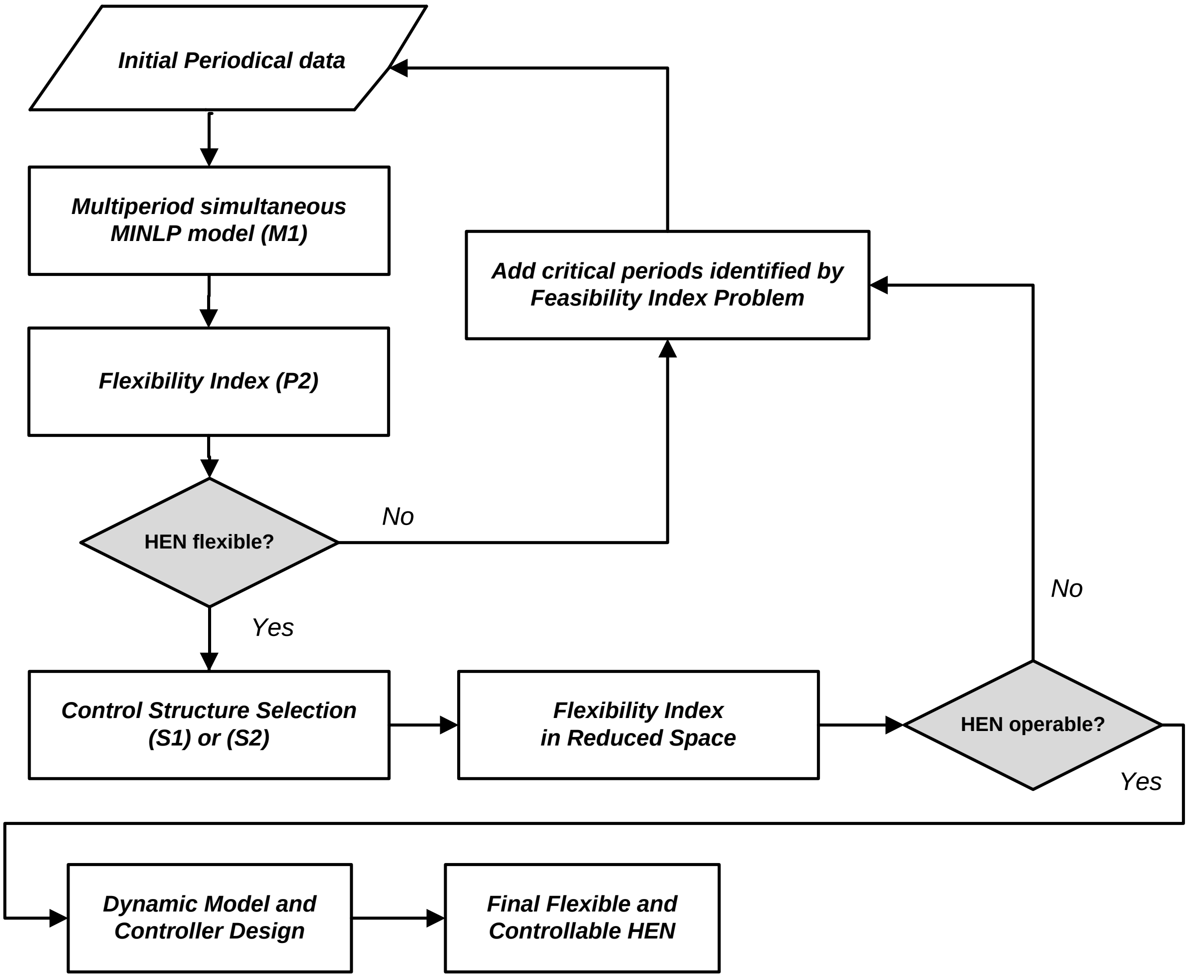


Figure 7.8: Outline of the solution strategy.

7.6 Numerical Examples

Three illustrative examples of simultaneous synthesis of multiperiod heat exchanger networks were solved. The MINLP models were formulated using GAMS and solve on an Intel Core 2.67 GHz machine with 2.96 GB memory. GAMS/CONOPT 3.0 was used to solve the NLP problems, GAMS/CPLEX 10.0 was used for the MILP problems, and GAMS/DICOPT was employed for solving the MINLP problems. The generation of the static and dynamic models, the controller design and simulations were made in Matlab.

7.6.1 Numerical Example 01

The first numerical example involves two hot streams and two cold streams. The nominal data for the problem is listed in Table 7.1. It is assumed expected variations in the inlet temperatures of $\delta_T = 10$K, a ΔT_{min} of 10 K and the minimum number of stages was set to two.

Table 7.1: Problem data for Example 1.

Stream	T_{in} (K)	T_{out} (K)	*F* (kW.K^{-1})	*h* (kW m^2 K^{-1})
H1	583±10	323	1.4	0.16
H2	723±10	553	2.0	0.16
C1	313±10	393	3.0	0.16
C2	388±10	553	2.0	0.16
CU	303	323		016
HU	573	573		0.16

Cost of Heat Exchangers (\$y^{-1}) = 5500+4333 [Area (m^2)]$^{0.6}$

Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})

Cost of Heating Utility = 171.428 (\$kW^{-1}y^{-1})

The example was solved for the nominal data using the model ($P1$) resulting in the design depicted in Figure 7.9 with a TAC of 92210 \$/y. The structure is well integrated since there is only one utility exchanger and no hot utility consumption.

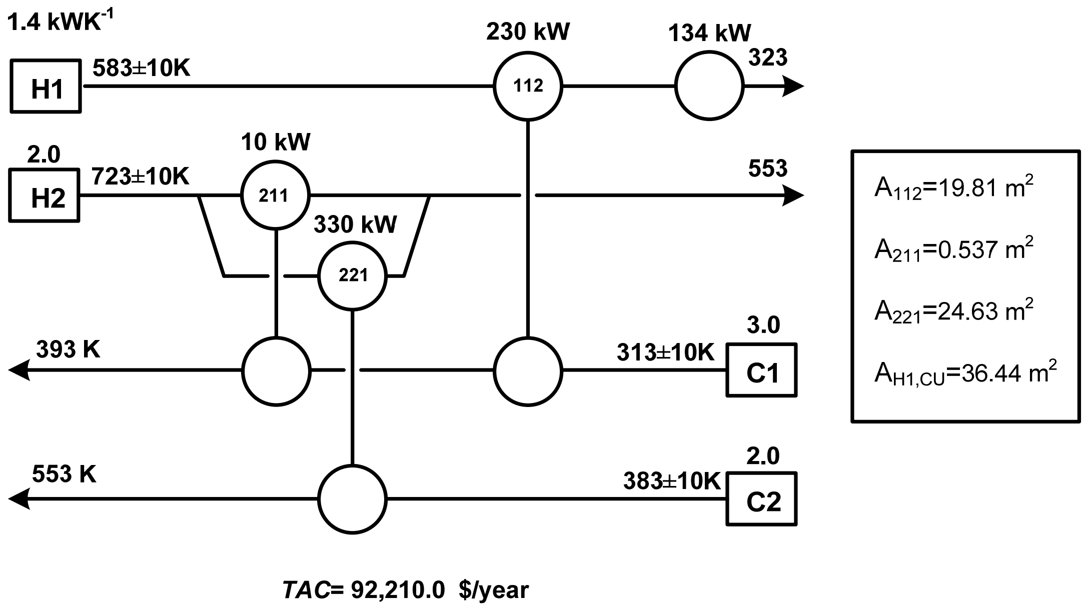


Figure 7.9: Nominal Design for numerical example 1.

For this example it is possible to generate the static model for disturbance propagation and control, i.e. the gain matrices for disturbances and for each potential manipulation (bypass on hot or cold side of each heat exchanger in the configuration). For the given heat load distribution a subroutine written in Matlab generates the following model:

$$
\begin{bmatrix} T_{H1}^{out} \\ T_{H2}^{out} \\ T_{C1}^{out} \\ T_{C2}^{out} \end{bmatrix} = \begin{bmatrix} 49.98 & 0 & 0 & 23.32 & 0 & 0 \\ -0.349 & 1.27 & 41.86 & -0.16 & 0.025 & 40.63 \\ -23.09 & -0.85 & 0 & -10.776 & -0.016663 & 0 \\ 0 & 0 & -41.86 & 0 & 0 & -40.63 \end{bmatrix} \begin{bmatrix} u_{112}^{H} \\ u_{211}^{H} \\ u_{221}^{H} \\ u_{112}^{C} \\ u_{211}^{H} \\ u_{221}^{C} \end{bmatrix}
$$

$$
+ \begin{bmatrix} 0.391 & 0 & 0.608 & 0 \\ 0.004 & 0.492 & 0.011 & 0.492 \\ 0.281 & 0.010 & 0.709 & 0 \\ 0 & 0.492 & 0 & 0.507 \end{bmatrix} \begin{bmatrix} T_{H1}^{in} \\ T_{H2}^{in} \\ T_{C1}^{in} \\ T_{C2}^{in} \end{bmatrix} \qquad (7.91)
$$

$$
+ \begin{bmatrix} 81.64 & 0 & -7.775 & 0 \\ 0.249 & 63.429 & -0.337 & -20.317 \\ 16.493 & 0.425 & -22.813 & 0 \\ 0 & 20.932 & 0 & -62.183 \end{bmatrix} \begin{bmatrix} F_{H1} \\ F_{H2} \\ F_{C1} \\ F_{C2} \end{bmatrix}
$$

With this model it is possible to estimate the impact of the disturbances on the controlled variables, and also select control structures with the best controllability properties based only on static knowledge. It is possible to notice that disturbances in the hot stream H2 and cold stream C2 will not affect the outlet temperatures of hot stream H1, since there is no downstream path pointed out by the zero gain. This is in accordance with the structured depicted in Figure 7.9. From the control structure point of view, only bypass on hot or cold side of heat exchanger between hot stream H2, cold stream C2 and stage 1 can be selected, since there are structural singularities from the other possible manipulations.

With the static model, the problem (S1) can be solved. Once the first structure was found, integer cuts were added in order to come up with all possible control structures, which minimize the overall interaction. A total of eight structures were found, all of them with RGA number of zero. Two possible control structures are shown in Figure 7.10.

For the nominal design, there is no control variables (n_z=0). Therefore all utility units must be used and all heat exchangers should be bypassed in order to control the network. For this particular case, there is no distinction between the Flexibility Index and the effective flexibility index, and a value of 0.25 was found pointing out that the design is not flexible enough in order to handle with the disturbance level. In fact, it is possible to say that the nominal designs can remain feasible only for variations of 2.5 K in the inlet temperatures, and a level of 10 K is required. The critical point identified at the solution of the problem ($P2$) is added to the nominal condition and the design is made again considering these two periods. The general results are listed in Table 7.2 and the periods considered in the design are given in Table 7.3. The TAC of the configuration is 130474 $/y and a Flexibility Index of 1.429. The configuration is depicted in Figure 7.11.

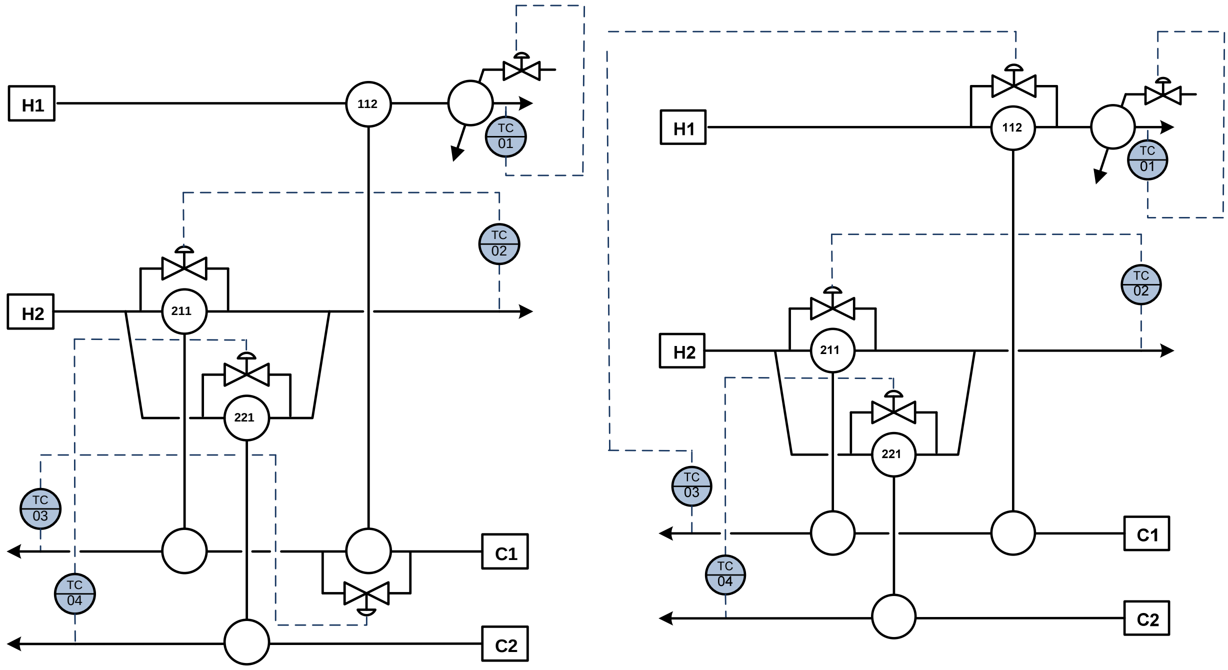


Figure 7.10: Two possible Control Structures for Nominal Design.

Table 7.2: General Results for TSS applied to Case Study 01.

$Iter.$	$Operating\ Cost\ (\$/y)$	$Investment\ Cost(\$/y)$	$Total\ Annual\ Cost\ (\$/y)$	$Flexibility\ Index$
1	8117	84093	92210	0.250
2	5573	124901	130474	1.429

Table 7.3: Uncertain Parameters for the Points considered.

$Iter.$	$T_{in}^{H1}(K)$	$T_{in}^{H2}(K)$	$T_{in}^{C1}(K)$	$T_{in}^{C2}(K)$
1	583	723	313	388
2	573	713	303	378

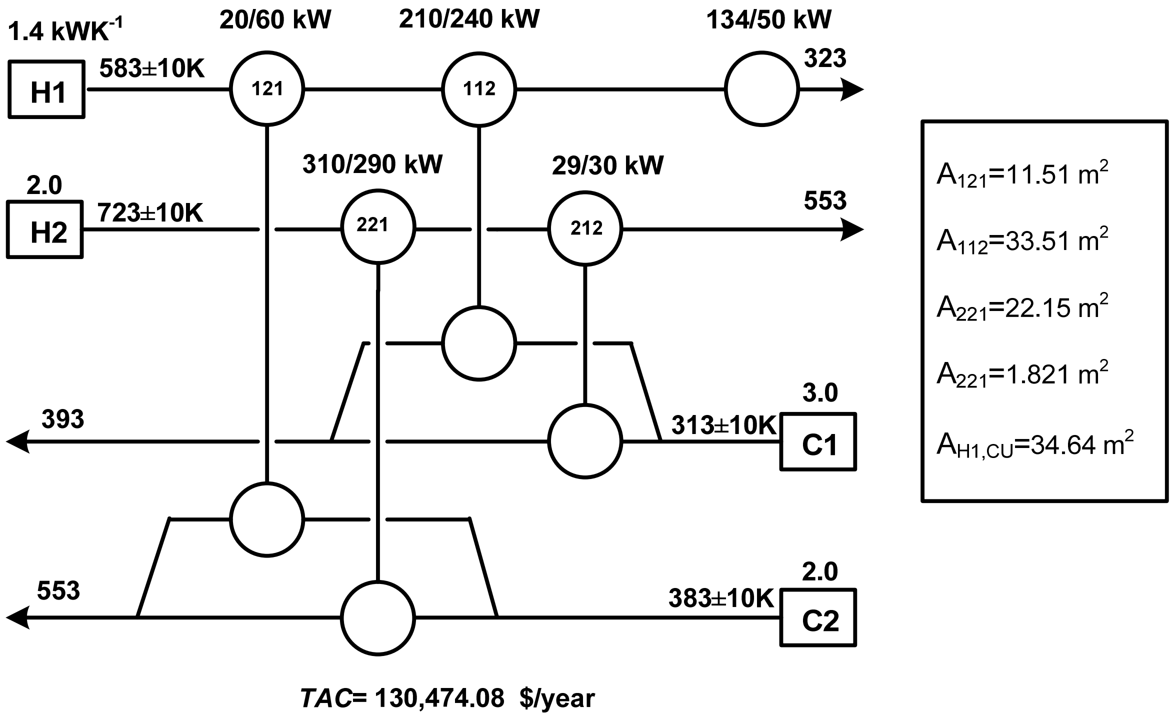


Figure 7.11: Final Configuration for Case Study 1.

$$
\begin{bmatrix} T_{H1}^{out} \\ T_{H2}^{out} \\ T_{C1}^{out} \\ T_{C2}^{out} \end{bmatrix} = \begin{bmatrix} 0.22 & 43.99 & 0 & 0 & 2.50 & 23.46 & 0 & 0 \\ 0 & 0 & 33.75 & 0.44 & 0 & 0 & 35.93 & 2.35 \\ 0.14 & -20.5308 & 1.401 & -0.29412 & 1.65 & -10.95 & 1.49 & -1.57 \\ -0.36 & 0 & -35.86 & 0 & -4.23 & 0 & -38.17 & 0 \end{bmatrix} \begin{bmatrix} u_{121}^{H} \\ u_{112}^{H} \\ u_{221}^{H} \\ u_{212}^{C} \\ u_{121}^{H} \\ u_{112}^{C} \\ u_{221}^{C} \\ u_{212}^{C} \end{bmatrix}
$$

$$
+ \begin{bmatrix} 0.383 & 0 & 0.586 & 0.030 \\ 0 & 0.506 & 0.058 & 0.435 \\ 0.253 & 0.021 & 0.687 & 0.038 \\ 0.051 & 0.463 & 0 & 0.486 \end{bmatrix} \begin{bmatrix} T_{H1}^{in} \\ T_{H2}^{in} \\ T_{C1}^{in} \\ T_{C2}^{in} \end{bmatrix}
$$

$$
+ \begin{bmatrix} 79.782 & 0 & -7.821 & -1.249 \\ 0 & 63.346 & -0.784 & -17.963 \\ 17.356 & 2.483 & -22.493 & -1.576 \\ 0.262 & 17.929 & 0 & -61.299 \end{bmatrix} \begin{bmatrix} F_{H1} \\ F_{H2} \\ F_{C1} \\ F_{C2} \end{bmatrix}
$$

Table 7.4: Effective flexibility index evaluation for each control structure.

Group	$Maniupulated\ Variables\ Subset$	Efective Flexibility Index
1	$\{q_{H1CU}\ \ u_{212}^{H}\ \ u_{112}^{H}\ \ u_{221}^{H}\}$, $\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{H}\ \ u_{221}^{H}\}$, $\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{C}\ \ u_{221}^{C}\}$, $\{q_{H1CU}\ \ u_{212}^{H}\ \ u_{112}^{C}\ \ u_{221}^{C}\}$, $\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{H}\ \ u_{221}^{C}\}$, $\{q_{H1CU}\ \ u_{212}^{H}\ \ u_{112}^{H}\ \ u_{221}^{C}\}$	0.733
2	$\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{C}\ \ u_{121}^{H}\}$, $\{q_{H1CU}\ \ u_{212}^{H}\ \ u_{112}^{C}\ \ u_{121}^{C}\}$, $\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{C}\ \ u_{121}^{C}\}$, $\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{H}\ \ u_{121}^{H}\}$	1.000
3	$\{q_{H1CU}\ \ u_{221}^{C}\ \ u_{112}^{C}\ \ u_{121}^{C}\}$	0.468

From the eleven control structures, one presents effective flexibility index (EFI) of 0.468, six present an EFI of 0.733 and only four are effectively flexible after the control structure is implemented with minimum RGA number. For each one of this four it was evaluated in addition the Condition Number, the minimum singular value and the disturbance sensitivity the results are listed in Table 7.5. As expected, all of them have the same level of interaction since the RGA number is zero. The minimum singular value must be the largest possible, so we can avoid problems with saturation, while the condition number and the disturbance sensitivity must be the lowest possible. According to these heuristics, among the control structures the control structure number three is the most promising. All these four control structures can be visualized in Figure 7.12.

Table 7.5: Controllability Evaluation for promising control structures.

	$Maniupulated\ Variables\ Subset$	RGA Number	Minimum Singular Value $\sigma(G(0))$	Condition Number	Disturbance Sensitivity
1	$\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{C}\ \ u_{121}^{H}\}$	0	2.3279	7.3585	35.3148
2	$\{q_{H1CU}\ \ u_{212}^{H}\ \ u_{112}^{C}\ \ u_{121}^{C}\}$	0	0.4410	25.1665	188.3454
3	$\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{C}\ \ u_{121}^{C}\}$	0	2.3278	4.8157	35.3148
4	$\{q_{H1CU}\ \ u_{212}^{C}\ \ u_{112}^{H}\ \ u_{121}^{H}\}$	0	2.3513	18.1388	35.3148

It would be possible compare the closed loop performance for each one in order to decide which one is the best. However the main focus here is just to show that the design can be implemented in practice, therefore, the dynamic model and controller design were performed only for the promising structure.

For the dynamic model it was assumed four cells and arithmetic mean temperature difference in order to represent the driving forces. The model is generated in Mat lab. For each control loop a Proportional Integral (PI) controller was designed through the approach proposed by Escobar (2006). In this approach, for each output is specified a closed loop performance in terms of rise time and maximum percentual overshoot allowed. With the specification of the closed loop performance and the model, it is determined algebraically the ideal controller, whose response on frequency domain is approximated by a response of a low order controller as a PID controller. As a systematic way, it was selected a closed loop performance two times faster than the open loop and an overshoot of 10%. The control loop design and its specifications are listed in Table 7.6.

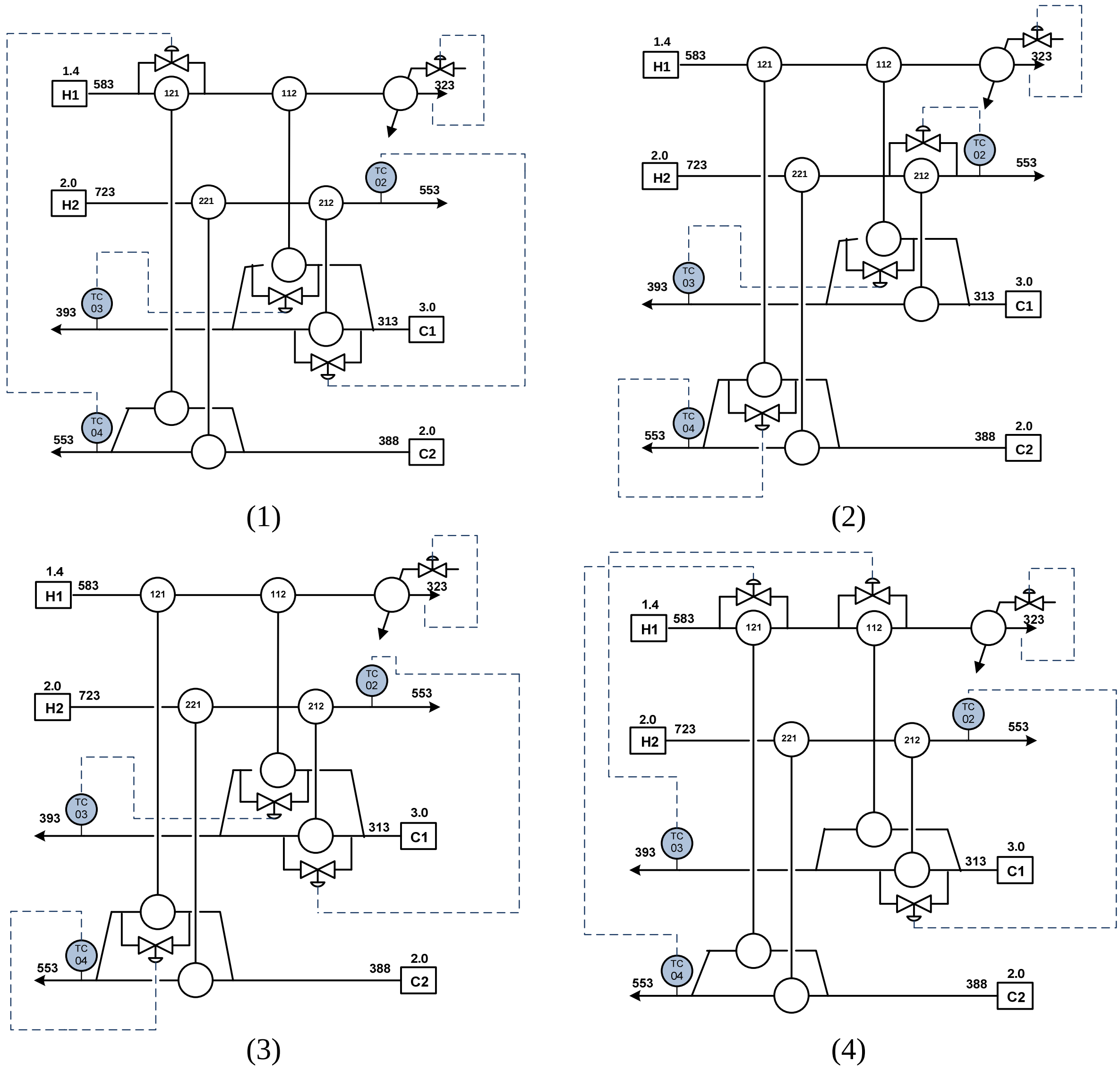


Figure 7.12: Four promisng control structures for Example 1.

Table 7.6: Control loop design for example 1.

Control loop	Controlled Variable (y)	Manipulated Variable (u)	Setpoint (y_{sp})	Manipulated Nominal Value (u_0)
1	T_{H1}^{out}	q_{H1CU}	323 K	134 kW
2	T_{H2}^{out}	u_{212}^{C}	553 K	0.4
3	T_{C1}^{out}	u_{112}^{C}	393 K	0.3
4	T_{C2}^{out}	u_{121}^{H}	553 K	0.2

In order to illustrate the closed loop performance some simulations were made. Initially was tested the servo response, i.e. the response to a setpoint change, since this is where for the design is made. The servo response for the first control loop is presented in Figure 7.13. When utility exchangers take place, they are the last exchanger providing a fast and direct effect on the outlet temperature. Moreover, with no interaction with the other control loops. These characteristics are very interesting for the control point of view. The main issue is that unfavorable disturbance direction can cause during the transient mode an increase in the utility consumption. However it is assumed that if a good and fast control is designed, most of the time during the operation the design will operate at nominal conditions, for which the total annual cost was minimized.

Another point to be considered is that since the control loop does not interact with others, it would be possible to design a controller as fast as we wish. However, disturbances in other streams may also remove the outlet temperature controlled by utility load from nominal conditions, a fast controller can implement more aggressive control actions in order to reject the disturbance and we must remember that the design is sufficiently flexible statically. The servo response for the control loop two is presented in Figure 7.14, for this particular there is a very low interaction with other loops. The servo response for the control loop 3, cause a disturbance in the control loop 1, but as can be seen in Figure 7.15, both loops achieve stationary conditions.

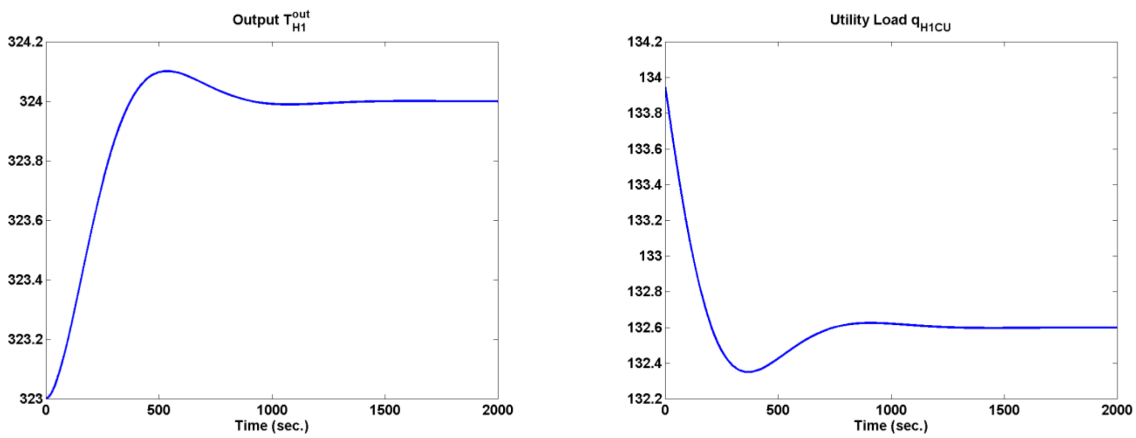


Figure 7.13: Servo Response for control loop 1.

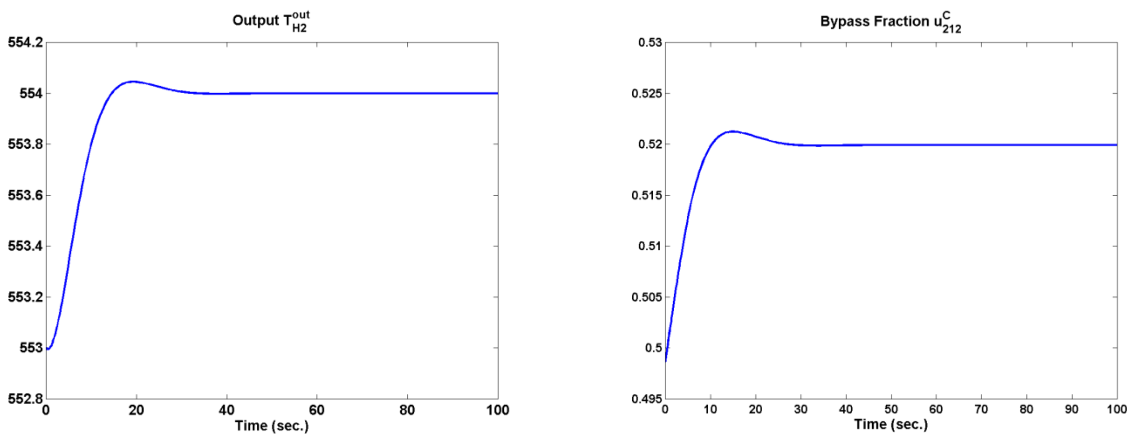


Figure 7.14: Servo Response for control loop 2.

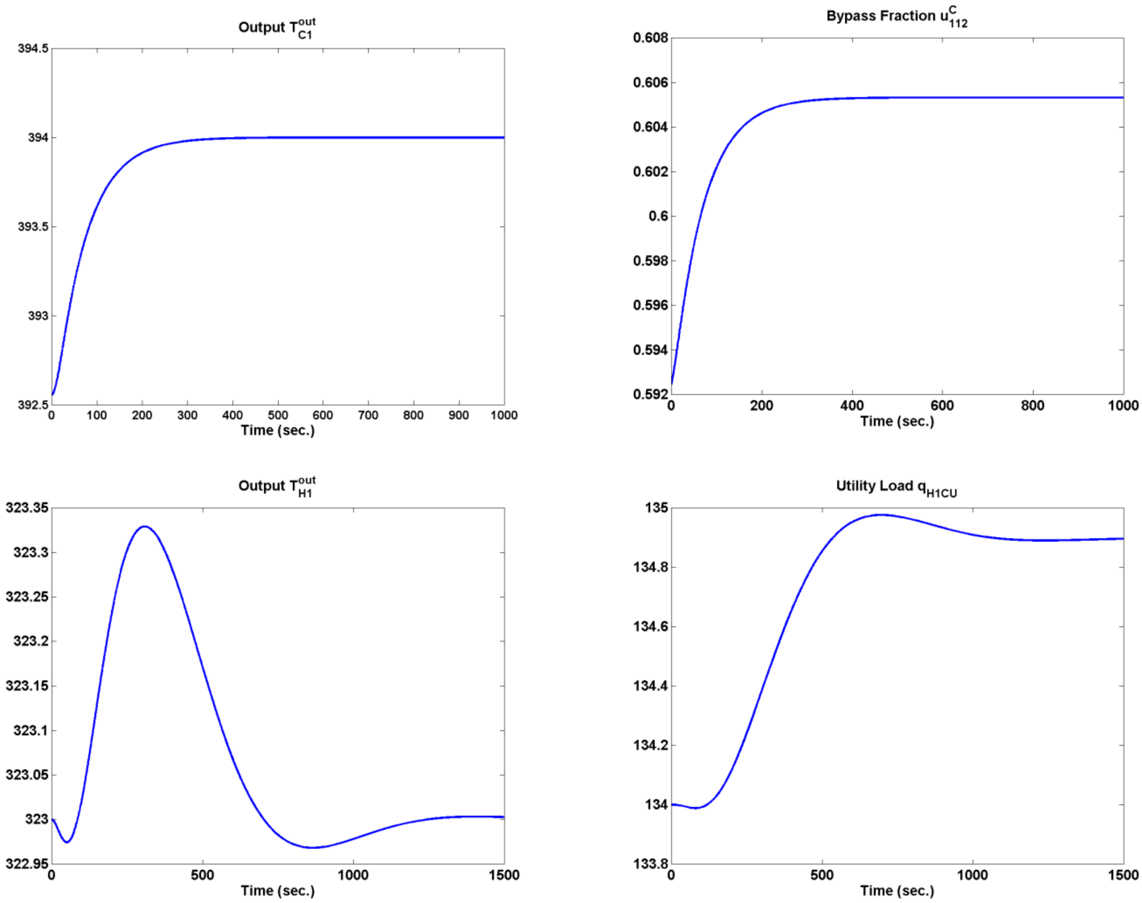


Figure 7.15: Servo response for control loop 3, and effect on loop 1.

The servo response for the control loop 4, cause a disturbance in the control loop 1 and 3, but as can be seen in Figure 7.16, both loops achieve stationary conditions.

The regulatory response was also tested in order to check the capability of the control system to reject disturbances. At the instant zero, all the inlet temperatures were increased of 10 K (step change) simultaneously. The response of each control loop is shown in Figure 7.17. It is possible to notice that the network can be controlled with this simple control structure. Additional improvements in the closed loop performance can be made testing different tuning parameters. The main idea was only to illustrate the satisfactory performance can be reached.

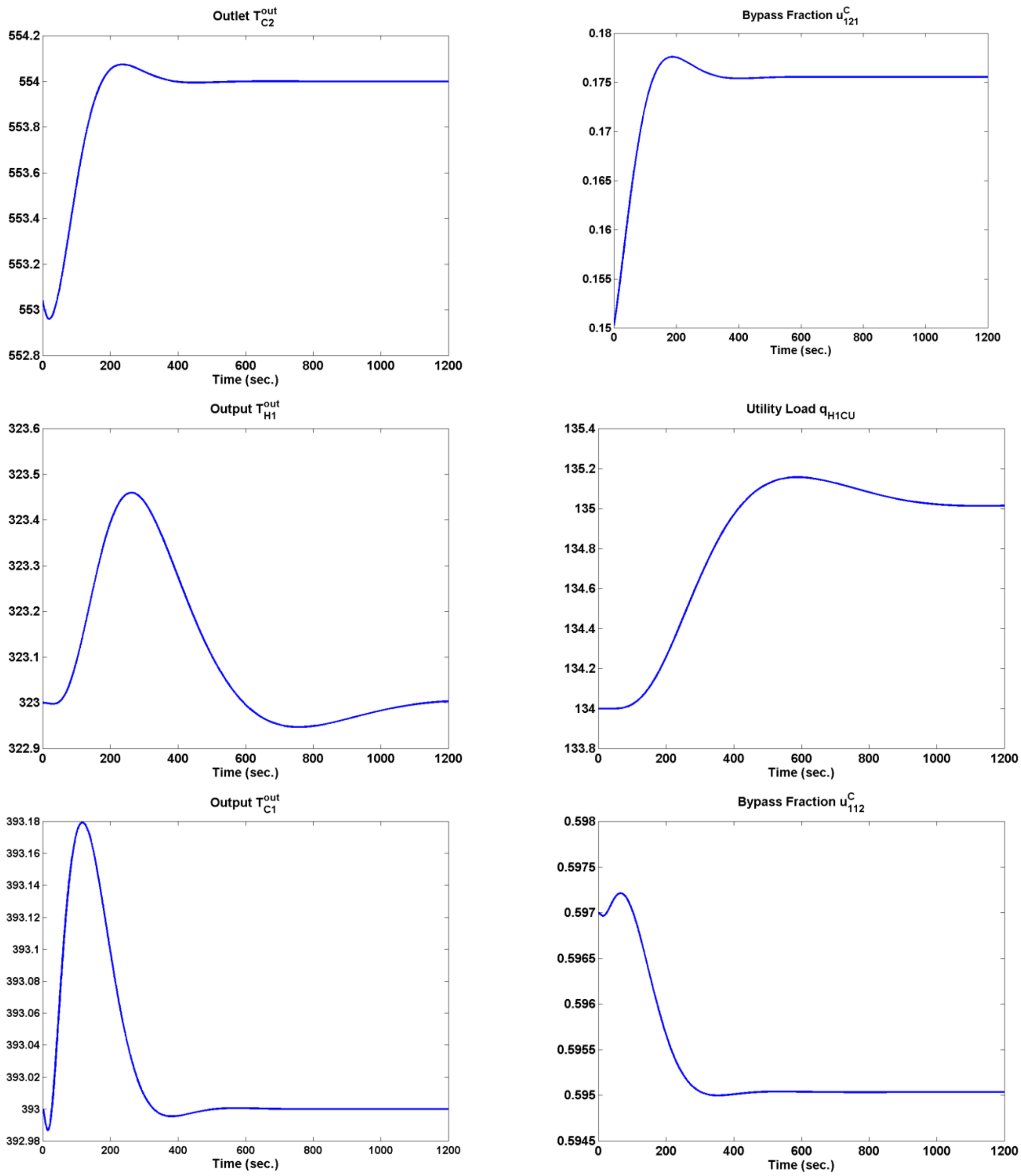


Figure 7.16: Servo response for control loop 4, and effect on loop 1 and 3.

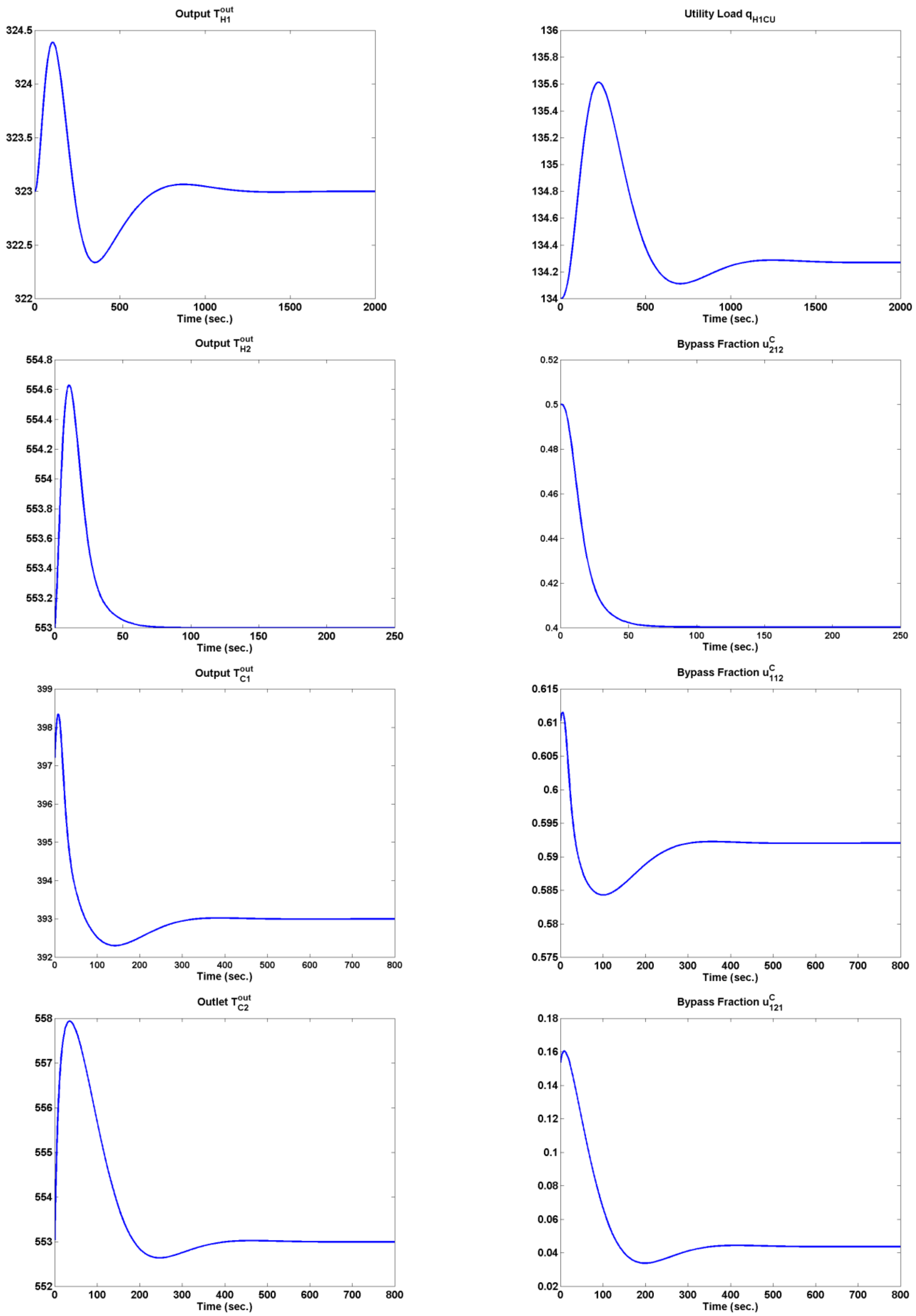


Figure 7.17: Regulatory response for all control loops for disturbance variation from nominal conditions to critical at instant zero.

7.6.2 Numerical Example 02

The second numerical example involves two hot streams and two cold streams. The nominal data for the problem is listed in Table 7.7. It is assumed expected variations in the inlet temperatures of $\delta_T = 10K$ for Hot stream H1 and $\delta_T = 5K$ for cold stream C2 and a variation of $\delta_F = 0.4$ in the heat capacity flowrates for both streams.

Table 7.7: Problem data for Example 2.

Stream	T_{in} (K)	T_{out} (K)	*F* (kW.K^{-1})	*h* (kW m^2 K^{-1})
H1	583±10	323	1.4±0.4	0.16
H2	723	553	2.0	0.16
C1	313	393	3.0	0.16
C2	388±5	553	2.0±0.4	0.16
CU	303	323		016
HU	573	573		0.16

Cost of Heat Exchangers (\$y^{-1}) = 5500+4333 [Area (m^2)]$^{0.6}$

Cost of Cooling Utility = 60.576 (\$kW^{-1}y^{-1})

Cost of Heating Utility = 171.428 (\$kW^{-1}y^{-1})

For this example it was generated a flexible design adding critical points identified as long as the design is not flexible. As presented in Table the final flexible design is found at fourth iteration with a TAC of 148515 \$/y and a Flexibility Index of 1.7134. The points considered at iteration are listed in Table 7.8 and the critical points described in Table 7.9.

Table 7.8: General results for flexible design for case study 2.

Iter.	*Operating Cost (\$/y)*	*Investment Cost(\$/y)*	*Total Annual Cost (\$/y)*	*Flexibility Index*
1	24758	67452	92210	0.1311
2	28823	96083	124905	0.1847
3	39540	92563	132194	0.6358
4	41749	106765	148515	1.7134

The design obtained is sketched in Figure 7.18. In order to make the design more flexible utility exchangers were added. For this final configuration it was generated the static model and different control structures were found. A comparative evaluation for controllability metrics are presented in Table 7.10. For this example, the control structure number two was selected for dynamic investigation and PI controllers were design for each control loop. The controller design and specifications for each control loop are listed in Table 7.11.

The increase of the number of streams, increase the number of nonlinear inequalities in the body of constraints making the Formulation 1 less robust to solve.

Table 7.9: Critical points considered until each iteration.

$Iter.$	T_{in}^{H1} (K)	f_{H1} (kW/K)	T_{in}^{C2} (K)	f_{C2} (kW/K)
1	583	1.4	388	2.0
2	593	1.8	383	2.4
3	593	1.8	393	1.6
4	573	1.0	383	2.4

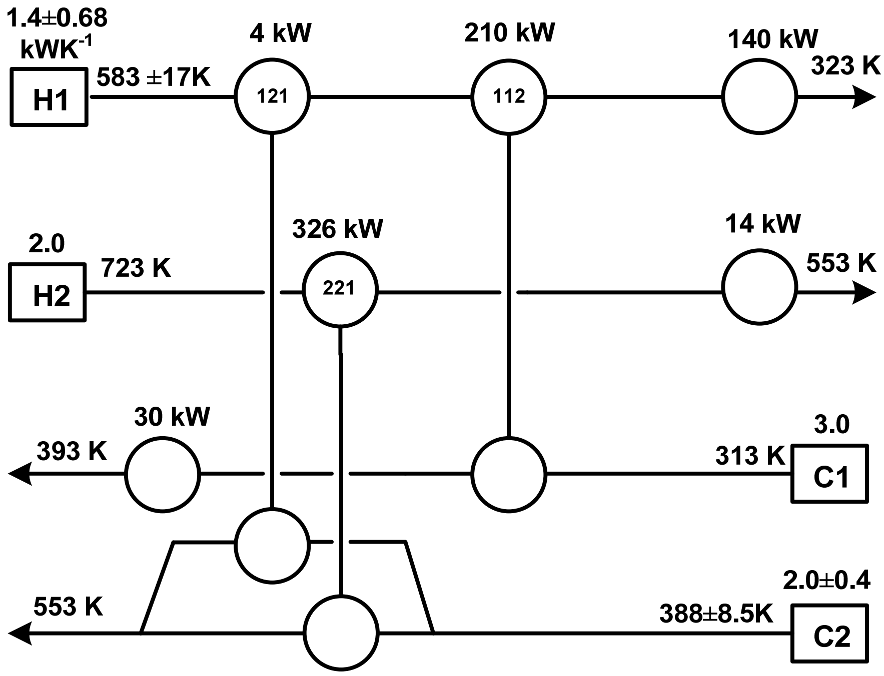


Figure 7.18: Flexible configuration for example 2.

Table 7.10: Controllability Evaluation for promising control strcutures.

	$Subset$	Rga Number	Min svd	Condition Number	Disturbance Sensitivity	Effective Flexibility
1	$\{q_{H1CU}\quad q_{H2CU}\quad q_{HUC1}\quad u_{121}^{H}\}$	0	0.3050	269.2436	430.5652	0.035
2	$\{q_{H1CU}\quad q_{H2CU}\quad q_{HUC1}\quad u_{221}^{H}\}$	0	0.3333	202.5701	444.5737	1.170
3	$\{q_{H1CU}\quad q_{H2CU}\quad q_{HUC1}\quad u_{121}^{C}\}$	0	0.3015	3.7091	307.1709	0.035
4	$\{q_{H1CU}\quad q_{H2CU}\quad q_{HUC1}\quad u_{221}^{C}\}$	0	0.3333	204.2359	346.6231	1.170

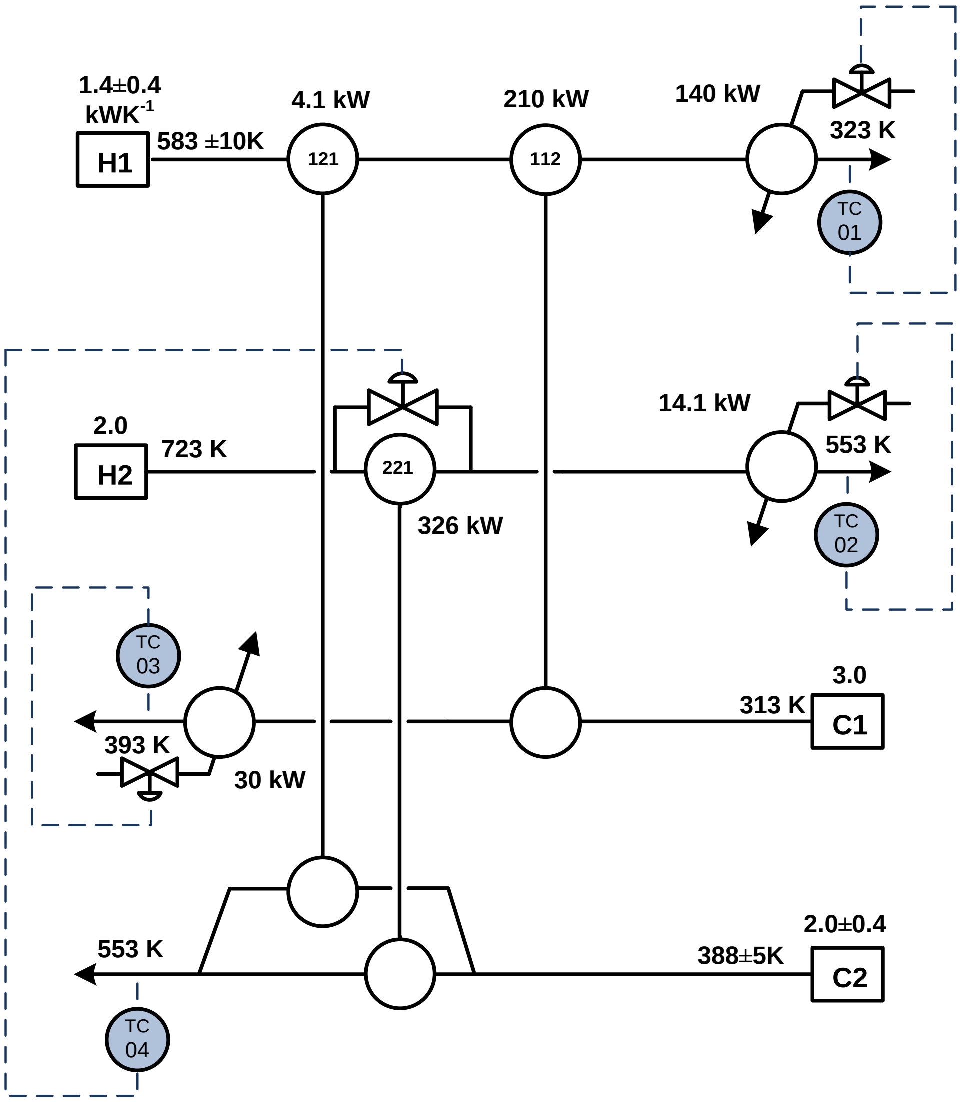


Figure 7.19: Final effective flexible design for example 2.

Table 7.11: Control loop design for example 2.

Control loop	Controlled Variable (y)	Manipulated Variable (u)	Setpoint (y_{sp})	Manipulated Nominal Value (u_0)
1	T_{H1}^{out}	q_{H1CU}	323 K	140 kW
2	T_{H2}^{out}	q_{H2CU}	553 K	14 kW
3	T_{C1}^{out}	q_{HUC1}	393 K	30 kW
4	T_{C2}^{out}	u_{221}^{H}	553 K	0.35

The servo response for the loops controlled by utility loads is presented in Figure 7.20, and the servo response for the fourth control loop and its effect are presented in Figure 7.21.

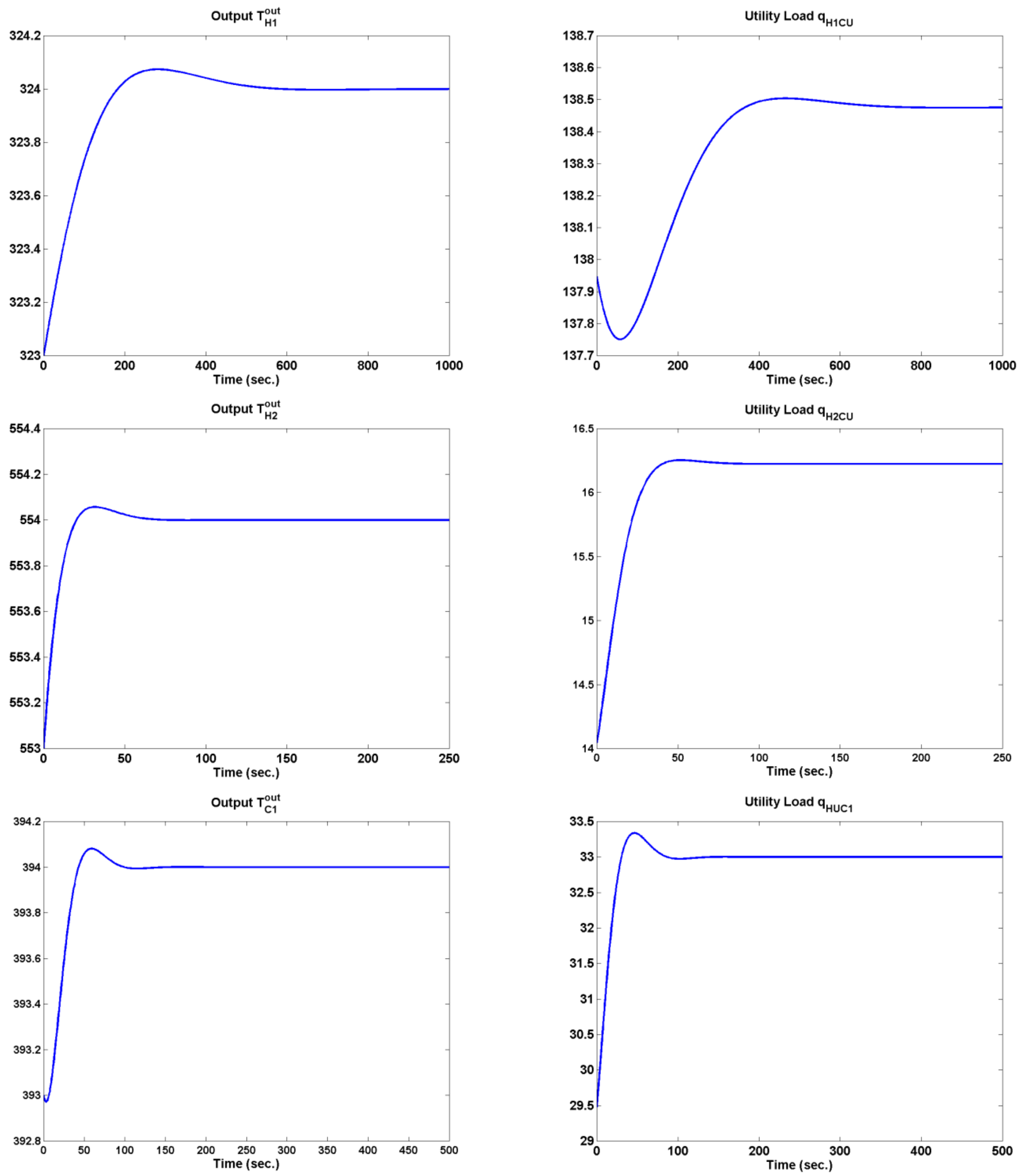


Figure 7.20: Servo response for the loops controlled by utility loads.

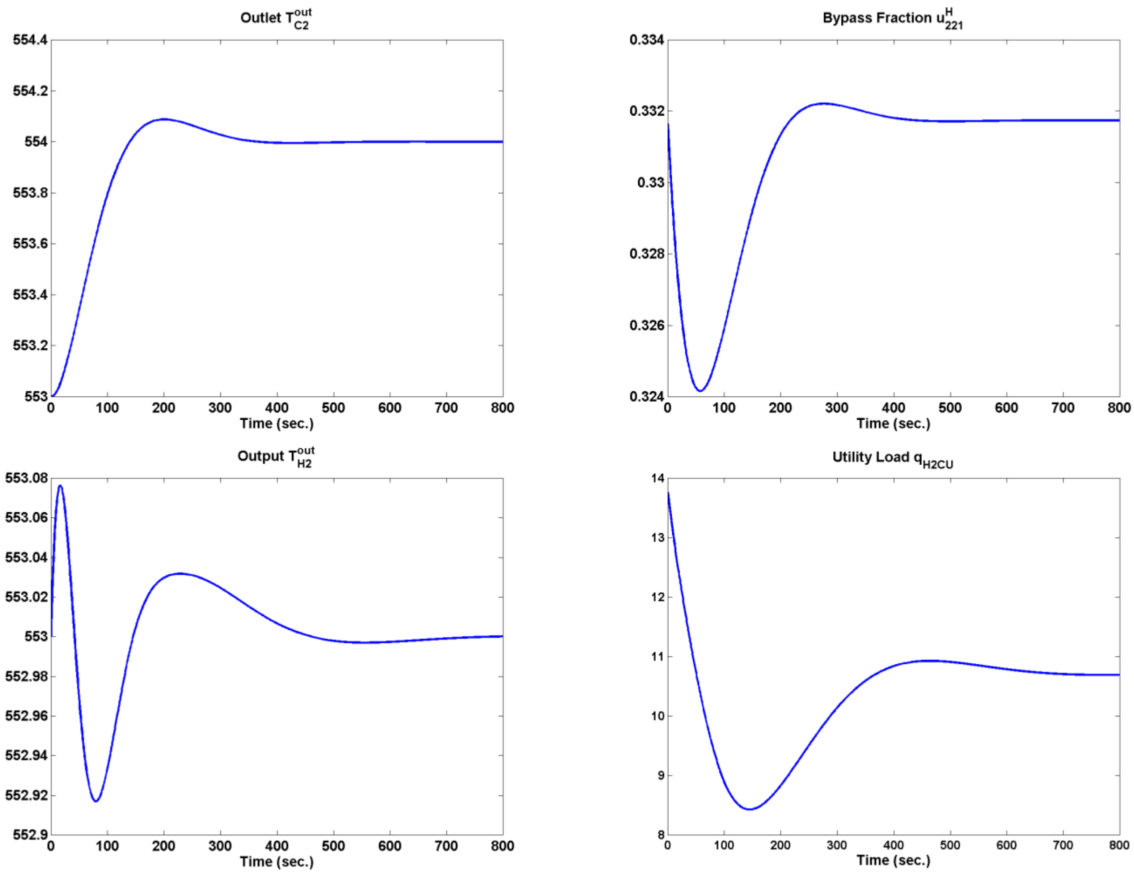
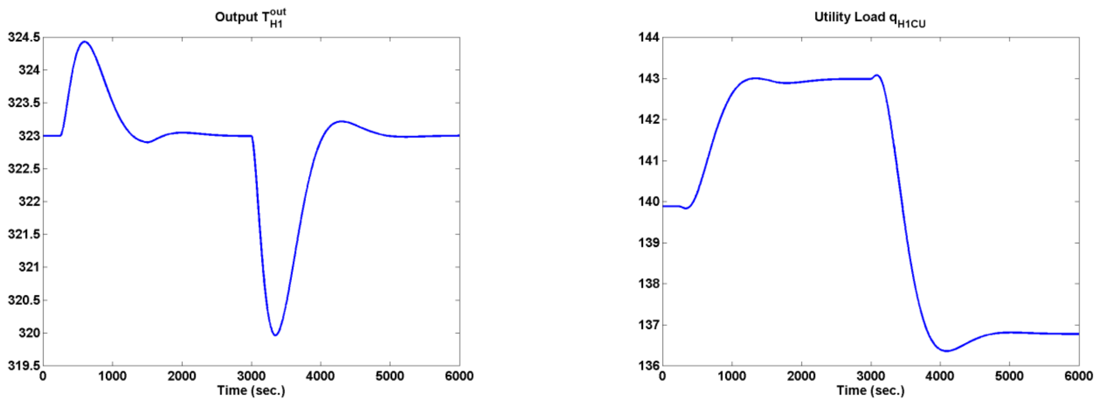


Figure 7.21: Servo response for control loop 4 and effect on control loop 2.

The regulatory response is presented in Figure 7.22. The simulation starts at nominal conditions, at 250 seconds occurs a step change to critical point 2, according to the Table 7.9. After that at 1500 seconds there is step change to critical point 3 and finally ate 3000 seconds a step change to critical point four in such way all critical points are considered. It is possible to notice that the control system can reject the disturbance level in a satisfactory way.



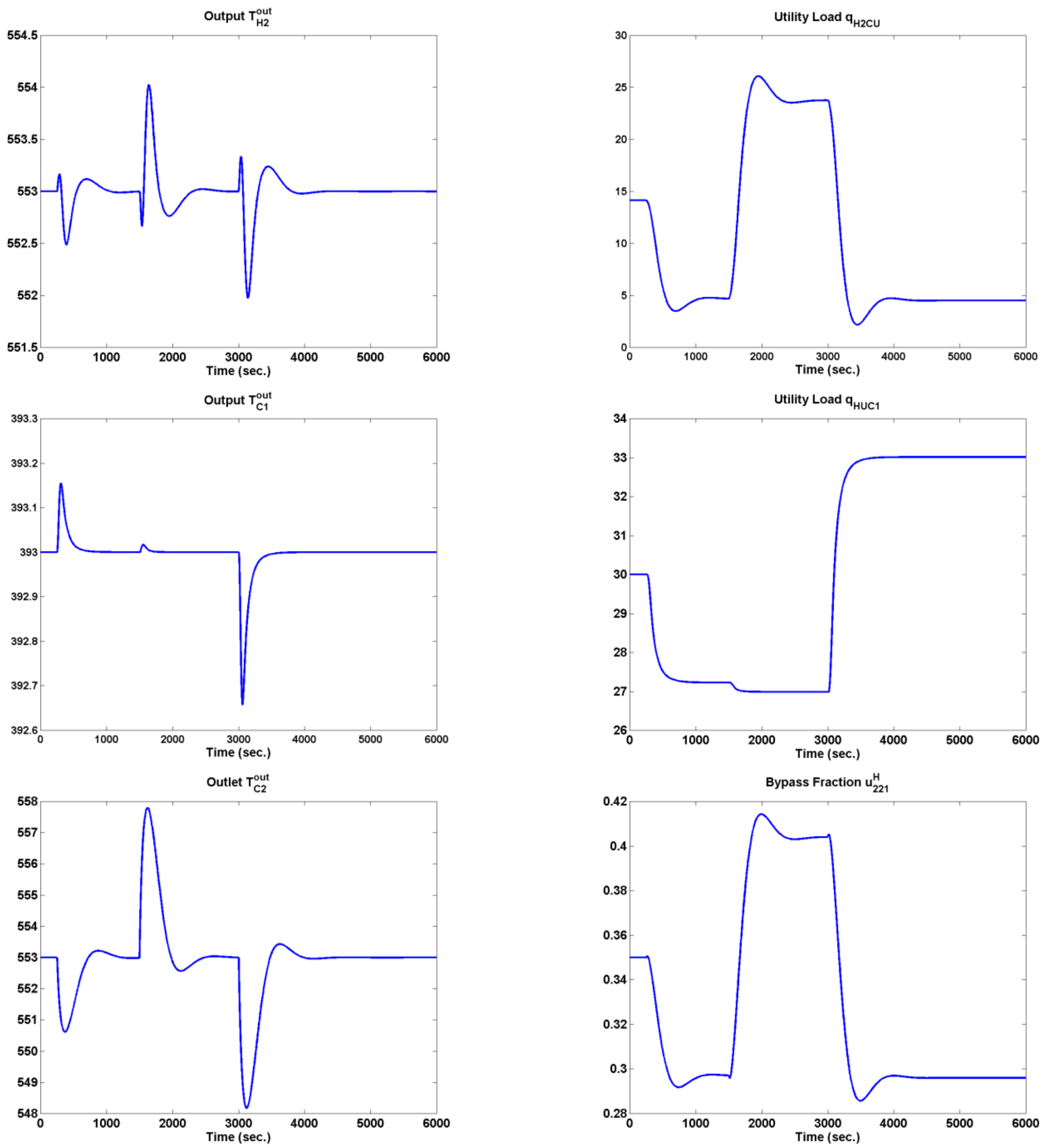


Figure 7.22: Regulatory response for all control loops, example 2.

7.6.3 Numerical Example 03

The third numerical example involves six hot streams and one cold streams. The nominal and economical data for the problem is presented in Table. It is assumed expected variations in the inlet temperatures of $\delta_T = 10K$ and a variation of $\delta_F = 5\%$ in the heat capacity flowrates. The minimum number of stages is set to 3.

The first design was generated with nominal condition. The flexibility index was 1.22 pointing out the flexible design; however the maximum effective flexibility index was 0.835. The critical point identified was all inlet temperatures dropped to -10K, the hot flowrates increase of 5% and the cold flowrates decrease of 5 % and then a second design is generated with a TAC of 975959 \$/y and a FI of 1.89. The general results are presented in Table 7.13.

Table 7.12: Problem data for example 3.

Stream	T_{in} (K)	T_{out} (K)	*F* (kW.K^{-1})	*h* (kW m^2 K^{-1})
H1	630±10	460	9.0±5%	1.2
H2	550±10	480	6.5±5%	0.6
H3	530±10	480	3.0±5%	0.4
H4	470±10	400	36.0±5%	0.6
H5	450±10	310	7.0±5%	0.4
H6	410±10	350	72.0±5%	0.4
C1	310±10	650	27.0±5%	1.2
CU	300	330		1.2
HU	700	700		0.3

Cost of Heat Exchangers (\$y^{-1}) = 100+866[Area (m^2)]$^{0.6}$

Cost of Cooling Utility = 52 (\$kW^{-1}y^{-1})

Cost of Heating Utility = 176 (\$kW^{-1}y^{-1})

Table 7.13: General results for flexible design for example 3.

Iter.	*Operating Cost* (\$/*y*)	*Investment Cost*(\$/*y*)	*Total Annual Cost* (\$/*y*)	*Flexibility Index*
1	755670.8	115079.5	870750.3	1.22
2	794478.8	181480.8	975959.8	1.89

For the second design, applying the same procedure as in the previous case studies the final configuration with the best control structure is depicted in Figure 7.23. The servo response for the design are presented in Figure 7.24 to 7.28. Finally, in Figure 7.29 is presented the regulatory response for a change from the nominal conditions to the critical point, where is possible to conclude that the design is flexible and controllable using the proposed approach.

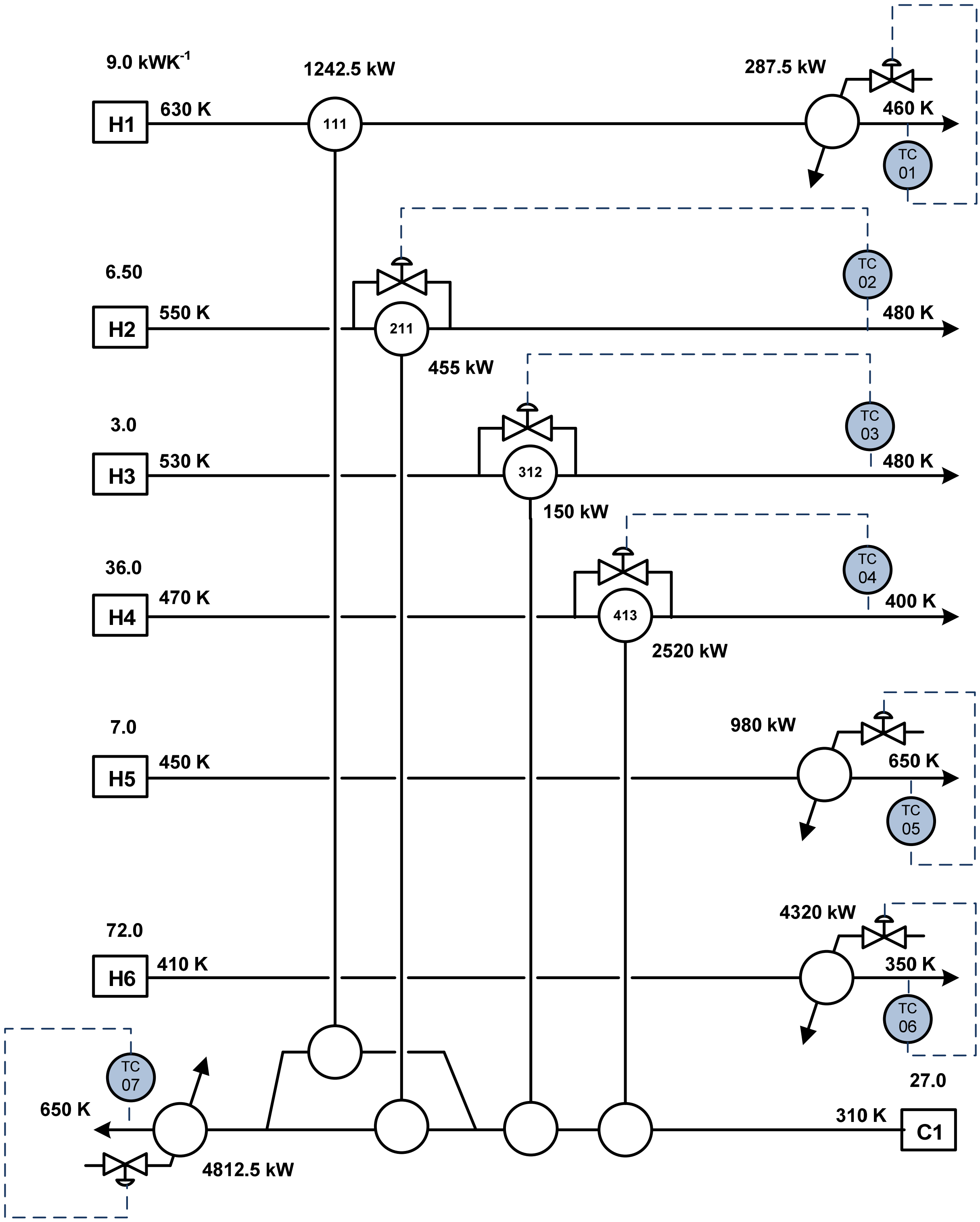


Figure 7.23: Final configuartion and control structure for the example 3.

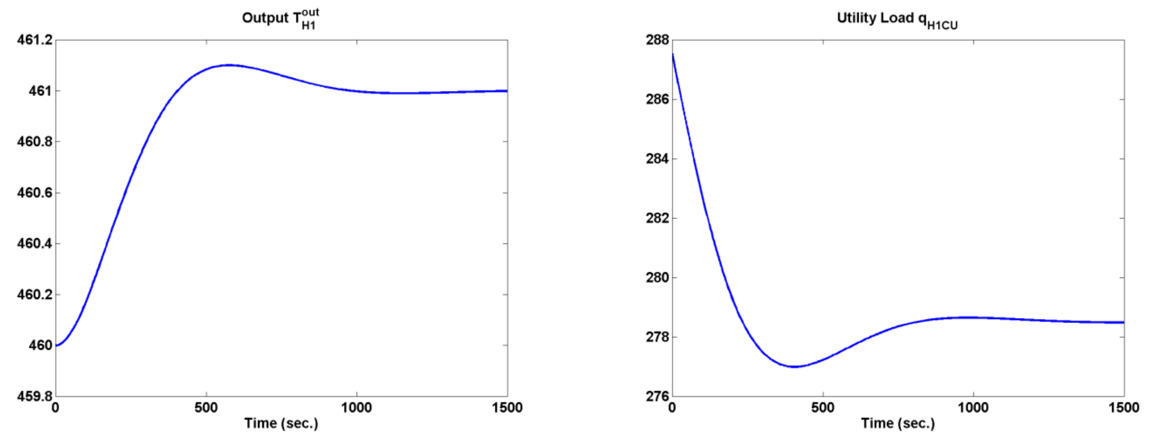


Figure 7.24: Servo response for control loop 1.

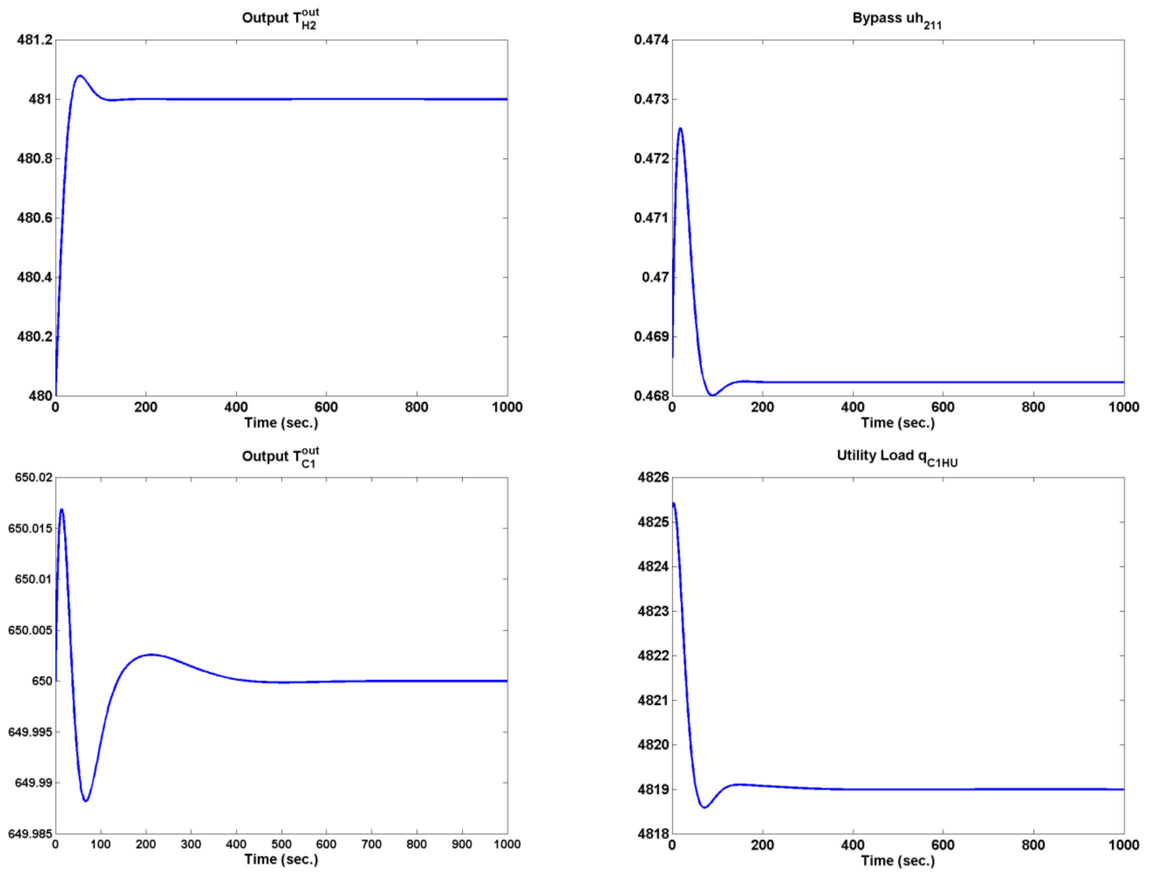


Figure 7.25: Servo response for control loop 2 and effect on control loop 7.

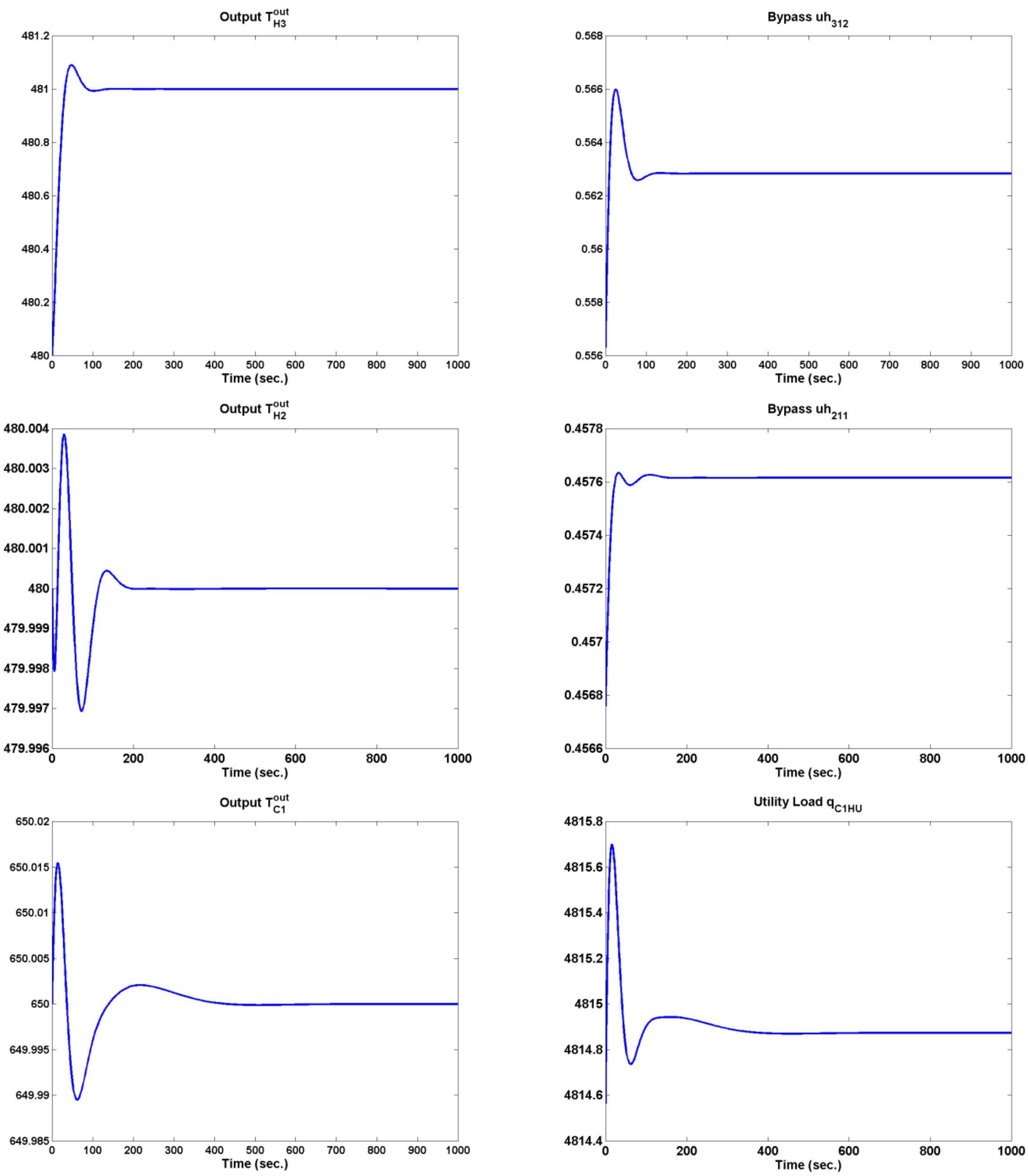
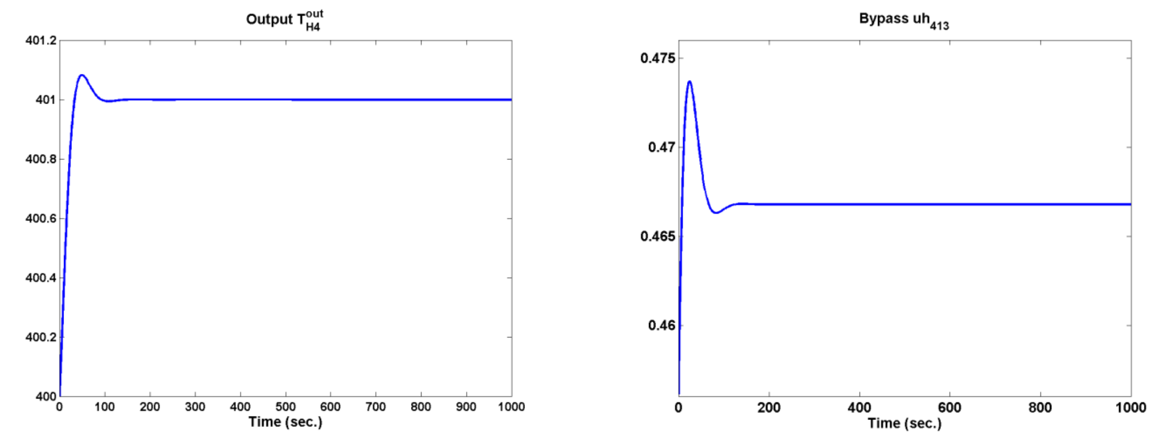


Figure 7.26: Servo response for control loop 3 and effect on control loop 2 and 7.



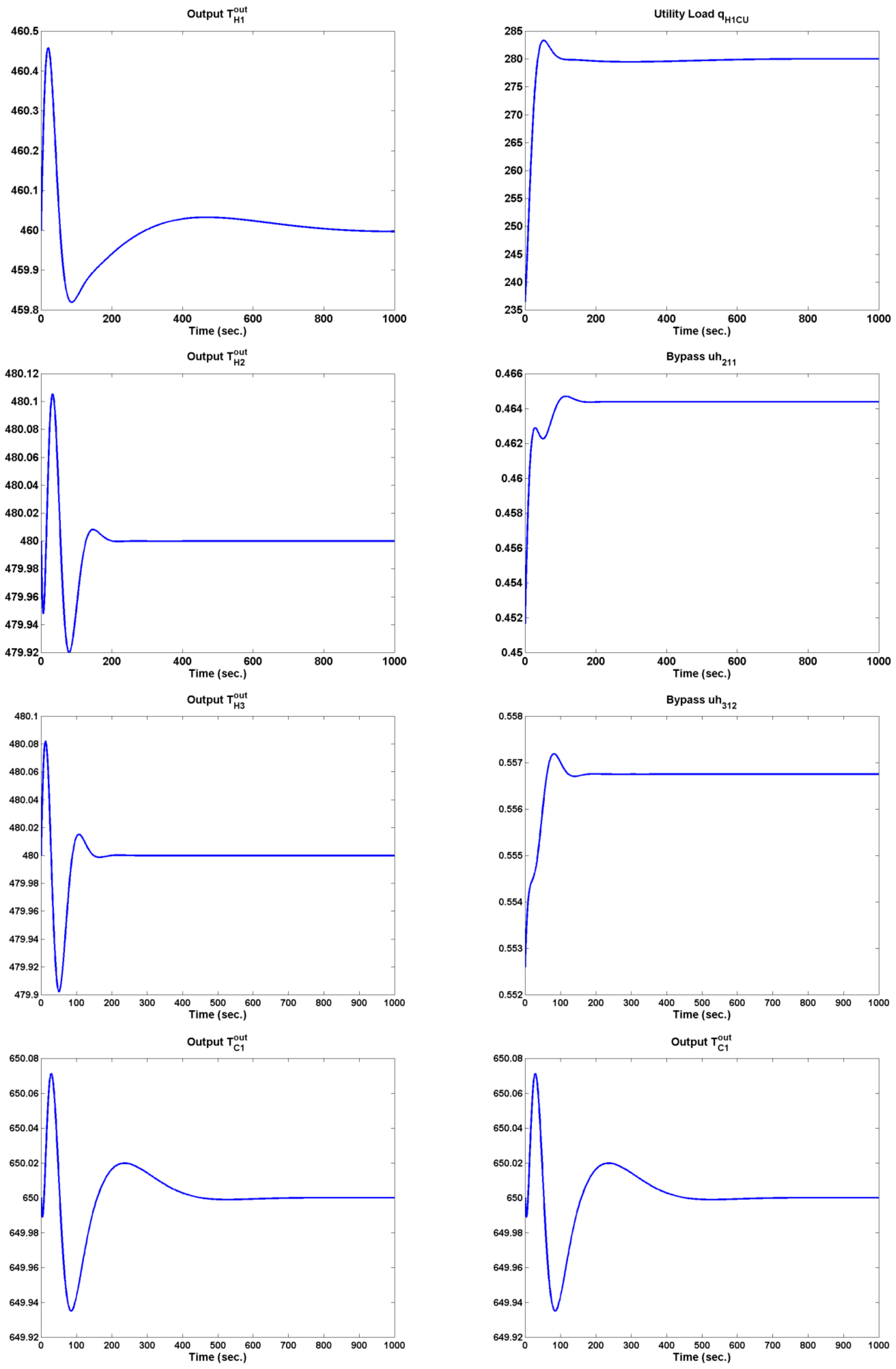
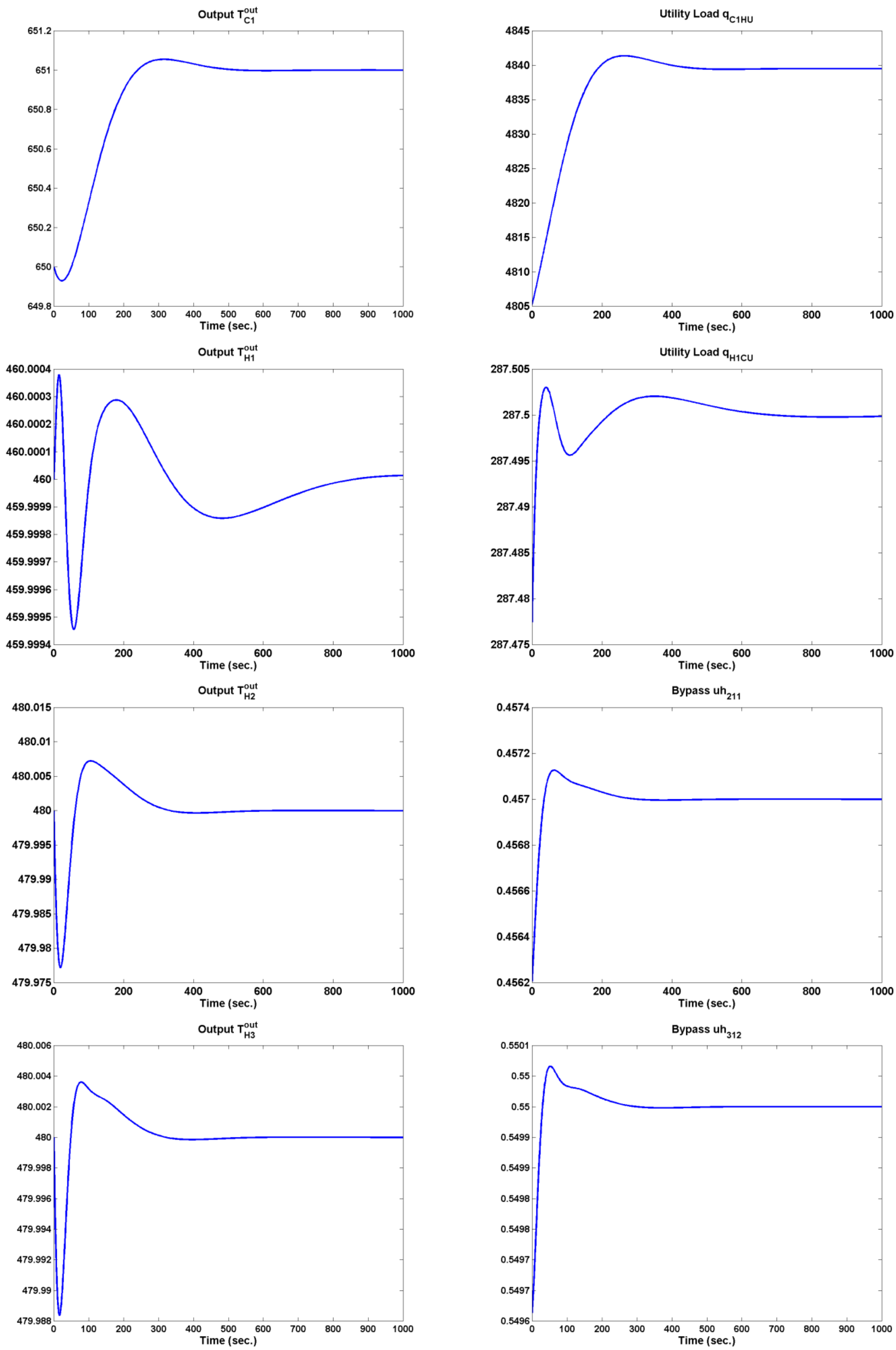


Figure 7.27: Servo response for control loop 4 and effect on control loop 1,2,3 and 7.


Output T_{C1}^{out}
Time (sec.)
Utility Load q_{C1HU}
Time (sec.)
Output T_{H1}^{out}
Time (sec.)
Utility Load q_{H1CU}
Time (sec.)
Output T_{H2}^{out}
Time (sec.)
Bypass uh_{211}
Time (sec.)
Output T_{H3}^{out}
Time (sec.)
Bypass uh_{312}
Time (sec.)

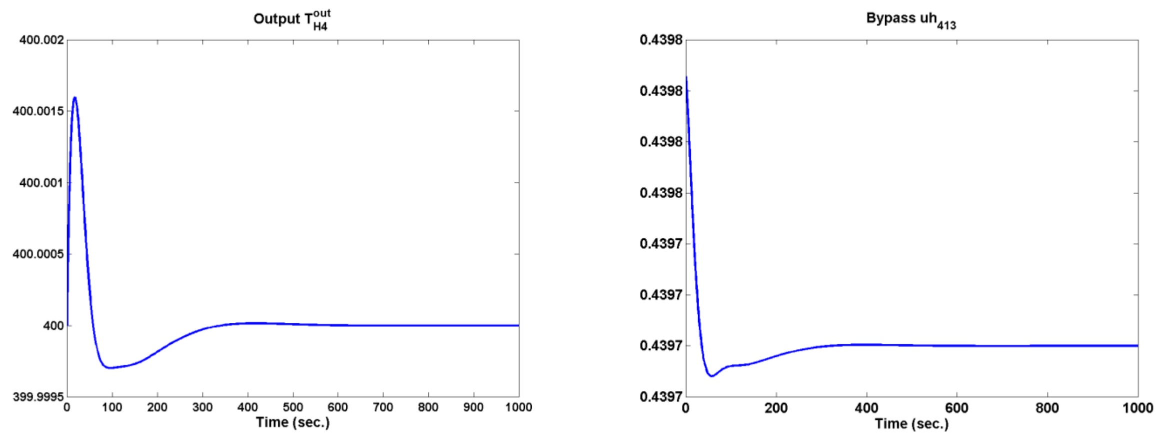
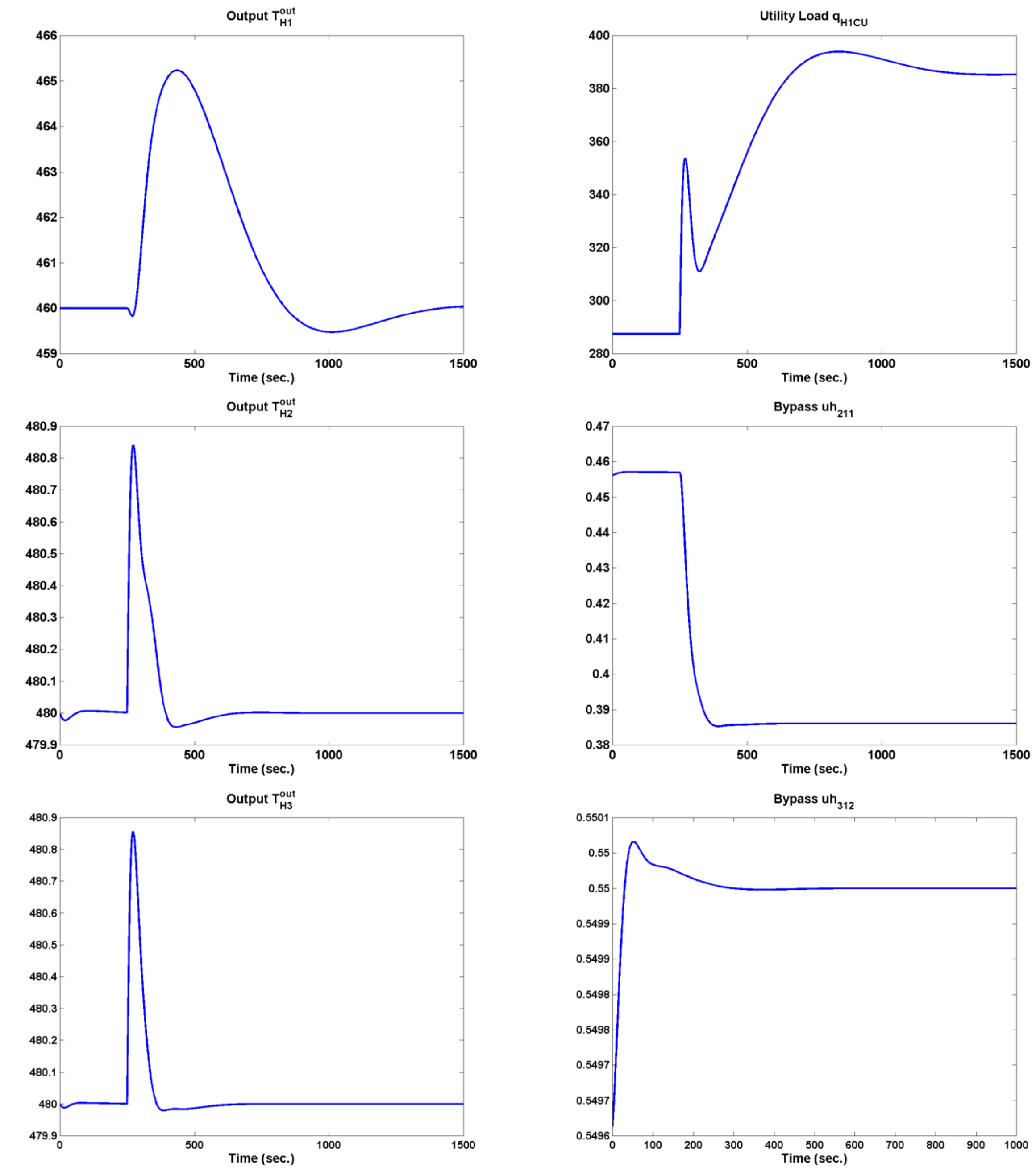


Figure 7.28: Servo response for control loop 7 and effect on control loop 1,2,3 and 4.



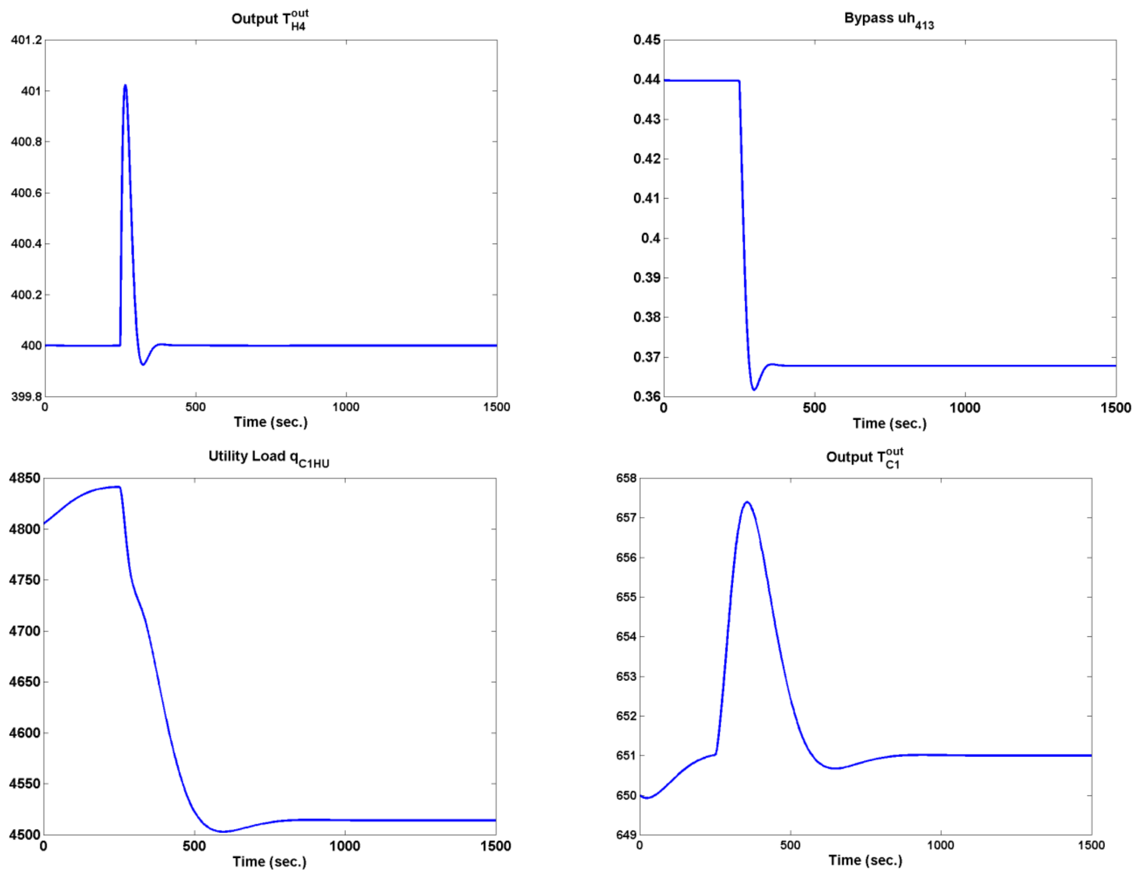


Figure 7.29: Regulatory response for all control loops, from nominal conditions to critical point 2 at 250 seconds.

7.7 Final Remarks and Conclusions

In this work the problem for design heat exchanger networks with operability considerations is addressed. First based on the two stage strategy it is possible to generate flexible designs. It was developed static and dynamic models for the networks that can generate automatically form the design stage. A MILP formulation is then used to give rise to the potential control structures and the closed loop performance is checked. Three numerical examples are used to illustrate the procedure.

Nomenclature

$Abbreviations$	
$EMAT$	*exchanger minimum approach temperature*
HEN	*heat exchanger network*
$HENS$	*heat exchanger network synthesis*
$LMTD$	*log mean temperature difference*
CSS	*control structure selection*
CS	*control structure*
FI	*flexibility index*
EFI	*effective flexibility index*
TAC	*total annual cost*

$Sets$	
CP	*set of cold process stream j*
CU	*set of cold utility*
HP	*set of hot process stream i*
HU	*set of hot utility*
CV	*set of controlled variables*
MV	*set of potential manipulated variables*
DV	*set of distrubance variables*
DV	
P	*set of periods*

$Variables$	$Units$	
d, x, z, θ		*vector of design, state, control and uncertain parameters respectively*
dt_{ijk}^{p}	[ºC]	*temp. approach between hot stream i, cold stream j, at location k and period p*
dt_{cui}^{p}	[ºC]	*temperature approach between hot stream i, and cold utility and period p*
dt_{huj}^{p}	[ºC]	*temperature approach between cold stream j, and hot utility and period p*
$LMTD_{ijk}^{p}$	[ºC]	*log mean temp. difference between hot stream i, cold stream j, at stage k*
$LMTD_{cui}^{p}$	[ºC]	*log mean temperature difference between hot stream i, and cold utility*
$LMTD_{huj}^{p}$	[ºC]	*log mean temperature difference between cold stream j, and hot utility*
$A_{i,j,k}$	[kW]	*area for heat exchanger between hot stream i and cold stream j at stage k*
$A_{cui,}$	[kW]	*area for heat exchanger between hot stream i and cold utility*
A_{huj}	[kW]	*area for heat exchanger between cold stream j and hot utility*
P_h	-	*Thermal effeciency*
$q_{i,j,k}$	[kW]	*heat load between hot stream i and cold stream j at stage k*
$q_{cui,}$	[kW]	*heat load between hot stream i and cold utility*

q_{huj}	[kW]	*heat load between cold stream j and hot utility*
q_{ijk}^{p}	[kW]	*heat load between hot stream i and cold stream j at stage k and period p*
q_{cui}^{p}	[kW]	*heat load between hot stream i and cold utility and period p*
q_{huj}^{p}	[kW]	*heat load between cold stream j and hot utility and period p*
t_{i}^{k}	[ºC]	*temperature of hot stream i at hot end of stage k*
t_{j}^{k}	[ºC]	*temperature of cold stream j at hot end of stage k*
$t_{i,p}^{k}$	[ºC]	*temperature of hot stream i at hot end of stage k and period p*
$t_{j,p}^{k}$	[ºC]	*temperature of cold stream j at hot end of stage k and period p*
s_j	-	*slack variable for constraint j*
u_h, u_c	-	*bypass fraction on hot side, cold side*
w_h, w_c	-	*heat capacity flowarte for hot side, cold side*

Binary Variables

$z_{i,j,k}$	-	*existence of the match between hot stream i, cold stream j, at stage k*
z_{cui}	-	*existence of the match between hot stream i, and cold utility*
z_{huj}	-	*existence of the match between cold stream j, and hot utility*

Parameters	*Units*	
$\beta_{i,j}$	-	*exponent for the area cost in exchanger i -j*
c	-	*cost for heat math between hot stream i and cold stream j*
ccu	[$/kW.yr]	*utility cost coefficient for cooling utility*
chu	[$/kW.yr]	*utility cost coefficient for heating utility i*
F_i, F_j	[kg/s]	*flow capacity of hot stream i, j*
h_i , h_j	[kW/m^{2}K]	*heat transfer coefficient for hot stream I,j*
T_i^{in}, T_j^{in}	[ºC]	*inlet temperature of hot stream i / cold stream j*
T_i^{out}, T_j^{out}	[ºC]	*outlet temperature of hot stream i / cold stream j*
δ	[ºC]	*expected variation for disturbance range*
Cp_h, Cp_c	[kW/KgK]	*Specific heat for hot/cold fluid*
ρ_h, ρ_c	[kg/m^3]	*mass density for hot and cold fluid*
V_h, V_c	[m^3]	*volume for hot/cold fluid flow*
ρ	-	*weigth factor*
φ	-	*disturbance sensitivity*
ΔT_{min}	[kW/K]	*minimimum temperature approach*
U_{ijk}	[kW/K]	*Global heat transfer coefficient*
Ω	[kW]	*upper bound for heat exchangers*

Γ	[ºC]	*upper bound for temperature difference*
μ	-	*lagrangean multipliers for*
λ	-	*lagrangean multipliers for*

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Capítulo 8

Conclusões e Considerações Finais

Síntese de redes de trocadores de calor consiste num assunto de grande interesse do ponto vista industrial, uma vez que envolve grande parte do custo de investimento e operacional de um processo. No entanto, a síntese convencional apresenta uma série de hipóteses simplificadoras, distanciando sua aplicabilidade de estudos de casos reais. Embora, soluções praticamente ótimas possam ser alcançadas utilizando técnicas apropriadas de otimização, sua transcrição para um cenário industrial requer que aspectos relativos à operação sejam considerados ainda na etapa de projeto.

Este trabalho teve como objetivo estudar o projeto e a operação de redes de forma a propor uma estratégia sistemática para síntese de redes de trocadores de calor capazes de operara sujeito a variação nas vazões e temperaturas e que possa ser implementado utilizando estratégias de controle convencionais.

No Capítulo 3, o problema da síntese e os principais métodos existentes na literatura, i.e. métodos sequenciais e simultâneos, foram avaliados. Pode-se verificar através da aplicação em cinco estudos de caso com diferentes dimensões que métodos simultâneos geram redes mais econômicas que os métodos sequenciais. Apesar dos modelos matemáticos de maior complexidade, a grande evolução em termos computacionais e desenvolvimento de novos algoritmos para MINLPs na última década permite essa realidade. A partir desse estudo verificou-se que o modelo SYNHEAT proposto por Yee e Grossmann (1990) apresenta um potencial promissor para possíveis extensões, tendo em vista que região viável do problema é linear, apresentando não linearidades somente na função objetivo.

O modelo SYNHEAT foi proposto em 1990 por Yee e Grossmann. Este modelo está baseado na postulação de uma superestrutura definida em estágios de troca térmica. Tendo em vista que o modelo SYNHEAT apresenta considerações que reduzem significativamente o número de estruturas contempladas na enumeração implícita através da superestrura, no Capítulo 4 foi realizado um estudo comparativo entre o modelo original e um modelo rigoroso que não considera as simplificações do modelo Synheat. Três estudos de caso foram resolvidos com os dois modelos. Foi evidenciado que com o modelo SYNHEAT é possível a obtenção de melhores soluções. Este estudo mostrou a importância do compromisso entre a acuracidade do modelo e a capacidade de obtenção de boas soluções.

Um dos grandes problemas na utilização de métodos de otimização para síntese de redes de trocadores de calor consiste na natureza combinatorial do problema que cresce exponencialmente com o número de correntes. Esta situação fica ainda mais crítica quando se leva em considerações diferentes cenários operacionais. No Capítulo 5 são apresentadas diferentes extensões multiperíodo baseada no modelo SYNHEAT e foi proposto um algoritmo baseado em decomposição Lagrangeana associada com regras heurísticas para obtenção de uma sequencia de soluções viáveis do problema, sem que para isso o problema seja resolvido o problema original de maior dimensionalidade. Através dessa proposição pode-se aumentar o tamanho do problema que podem ser tratados com a sistemática proposta nesse trabalho.

No Capítulo 6 é apresentado o procedimento em dois estágios para o desenvolvimento de redes com determinado grau de flexibilidade. Este procedimento é iterativo onde são resolvidos sequencialmente um problema multiperíodo e uma análise de flexibilidade que visa identificar pontos críticos que devem ser adicionados para que o projeto seja realizado novamente.

No Capítulo 7 é apresentada a metodologia proposta neste trabalho. Assumiu-se um projeto de controle descentralizado utilizando controladores de baixa ordem, por serem simples de implementar e altamente difundidos no cenário industrial. Baseado na metodologia em dois estágios apresentada no Capítulo 6, foi proposta uma modificação, onde para o "*design*" proveniente do problema multiperíodo, são levantadas as estruturas de controle potenciais. Esta etapa se dá através da solução de um problema MILP e passa pela geração das matrizes de ganho para o sistema em estudo. Uma vez selecionada estrutura de controle é calculado o índice de flexibilidade efetivo, com a limitação imposta pela estrutura de controle, e os possíveis pontos críticos são adicionados ao problema multiperíodo para que seja feito o projeto da estrutura. Por fim, simulações dinâmicas permitem avaliar o comportamento em malha fechada. Estudos de caso foram apresentados, evidenciando a aplicabilidade da metodologia proposta para o projeto de redes de trocador de calor que sejam capazes de operar para uma determinada faixa de incerteza nas vazões e temperaturas de entrada e que sejam possíveis de operar utilizando uma estrutura de controle simples e eficiente.

De maneira geral as principais contribuições desse trabalho foram: (*i*) o desenvolvimento de uma biblioteca de modelos em GAMS para síntese de redes; (*ii*) o desenvolvimento de uma biblioteca de modelos estáticos e dinâmicos para redes de trocadores de calor; (*iii*) implementação sistemática da metodologia em dois estágios para projeto de unidades flexíveis orientado ao modelo Synheat; (*iv*) desenvolvimento de algoritmo que associa decomposição lagrangeana com regras heurísticas para solução do problema multiperiodo em larga escala; (*v*) a sistematização do calculo do índice de flexibilidade para o modelo em estudo; (*vi*) e por fim, desenvolvimento e um metodologia para projeto da rede flexíveis e controláveis com controladores descentralizados.

8.1 Sugestões para Trabalhos Futuros

A metodologia apresentada nesse trabalho, embora considerada satisfatória em relação a proposta original, apresenta também limitações e particularidades de forma que algumas melhorias e extensões podem ser vislumbradas. Considerações como mudança de fase nas correntes de processo, e aplicação para o caso de "*retrofit*" (reprojeto) de unidades existentes seriam as mais emergentes. Esse tema tem sido abordado na literatura para o caso nominal. Extensões consideradas menos imediatas seriam a consideração da perda de carga, incerteza nos coeficientes de trasnferência de calor e o projeto detalhado dos trocadores de calor.

Em temos de metodologia, um estudo interessante consiste em realizar simultaneamente a seleção da estrutura de controle e a avaliação da flexibilidade efetiva num único MI(N)LP, uma vez que existe um compromisso entre a flexibilidade e a controlabilidade, uma vez definido o custo da rede na etapa de projeto. Esta implementação evitaria que diversas estruturas de controle fossem levantadas em uma etapa para possível avaliação da flexibilidade efetiva, reduzindo o tempo gasto no projeto. Outro aspecto a ser melhorado na metodologia consiste em selecionar estrutura de controle baseado em outras métricas de controlabilidade, inclusive dinâmicas, sendo o principal desafio formular o problema de maneira a evitar o máximo possível as não convexidades.

Como alternativa em termos de projetar redes com alta operabilidade, heurísticas podem ser adicionadas ao projeto. Estas heurísticas podem ser convertidas facilmente em proposições lógicas, que por sua vez são formuladas sistematicamente como inequações lineares, podendo ser adicionadas ao modelo. Por exemplo, evitar projetos com "*splits*", ou mesmo com poucos "*splits*" uma vez que estes podem causar efeitos concorrentes e, consequentemente resposta inversa. Ainda, evitar recombinação de correntes em diferentes estágios, pois poderia acarretar em perda de graus de liberdade. Pode-se ainda considerar uma restrição adicional para limitar o número de trocadores, tendo em vista que quanto menos trocadores, menos os distúrbios se propagam na rede, pela diminuição natural dos "*downstream paths*". De maneira geral, as heurísticas devem ser adicionadas e comparadas o custo refrente a ao projeto com ou sem heurística para que se possa verificar se os compromissos justificam ou não a adição da restrição (decisão essa que cabe ao projetista).

De maneira geral, os procedimentos foram implementados de forma sistemática. Foi feito um esforço no sentido de automatizar a geração dos modelos bem como a transmissão de dados de um passo para outro. Duas principais ferramentas foram utilizadas, GAMS e MATLAB. Visando a possibilidade de permitir que engenheiros possam utilizar a metodologia em suas diversas etapas foi criado um protótipo de uma interface para um "*toolbox*" em MATLAB que pode ser visualizada nas Figuras 8.1, 8.2 e 8.3.

Por fim, a metodologia proposta nesse trabalho foi orientada para HENS, no entanto, em termos teóricos pode ser estendida para aplicação em redes de integração mássica, ou mesmo para o projeto de reatores, redes de reatores e projeto e sequenciamento de colunas de destilação.

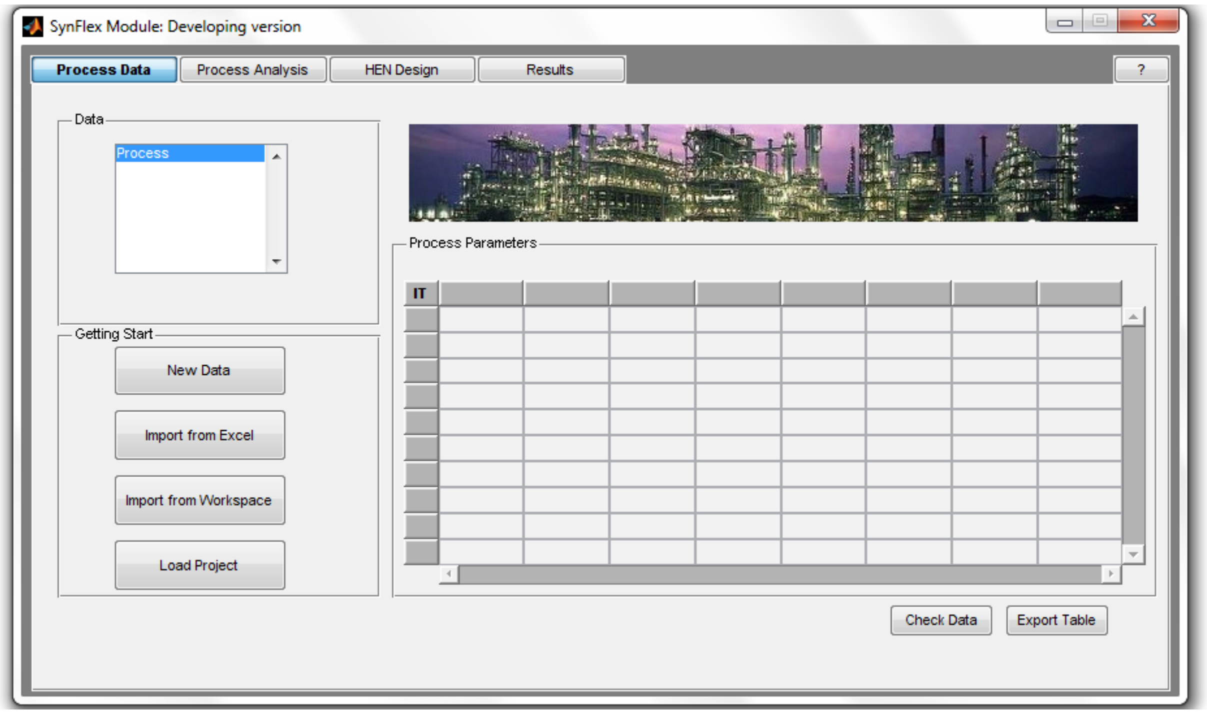


Figura 8.1: Interface inicial do SynFlex Toolbox para Matlab.

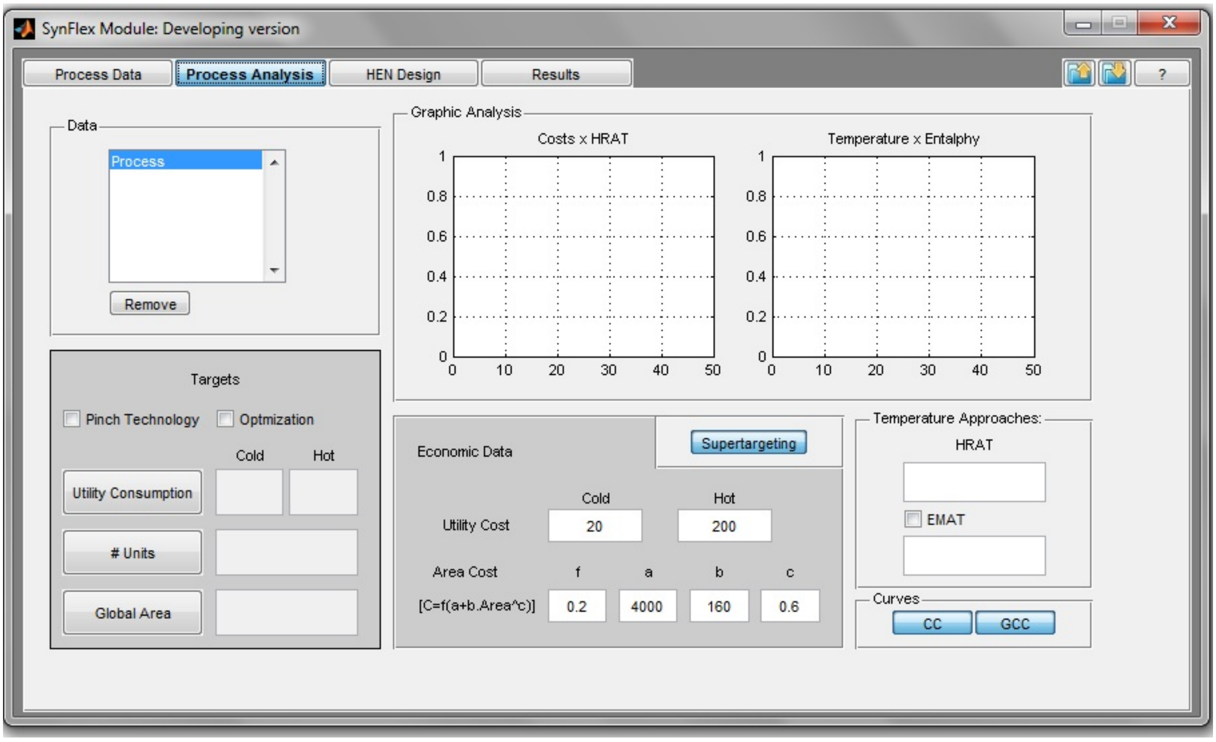


Figura 8.2: Interface de análise do SynFlex Toolbox para Matlab.

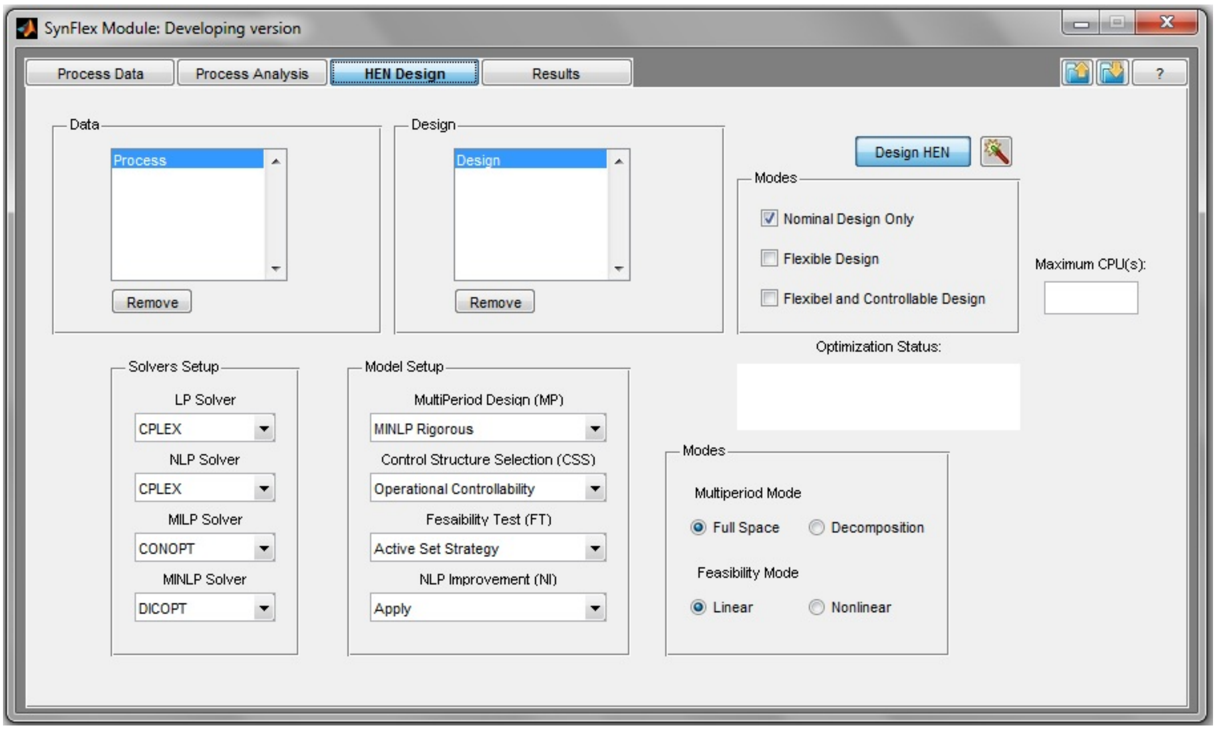


Figura 8.3: Interface de projeto do SynFlex Toolbox para Matlab.

É possível destacar como ponto forte do trabalho a automação dos procedimentos, que embora tenham caratér apenas acessorial, foi bastante dispendioso. Este trabalho contou com a colaboração do Prof. Ignácio Grossmann, cujo trabalho é considerado pioneiro em Síntese de Redes de Trocadores de Calor utilizando otimização. Acredito que essa colaboração foi fundamental para a implementação, entendimento e interpretação dos modelos.

Esperava-se um procedimento totalmente simultâneo, onde todos os compromissos seriam considerados num único MINLP. Grande esforço foi feito no sentido de escrever genericamente o modelo linearizado baseado na superestrutura. Com o aprofundamento teórico foi se percebendo que é tentador adiconar restrições a um problema de otimização, no entanto, conforme exemplificado no Capítulo 4, o modelo resultante não tem grande valia se não podemos extrair dele bons resultados. É necessário, reformular, aproximar, decompor, dentre outras operações para que se consiga utilizar o potencial dos métodos matemáticos. Por fim, este trabalho foi realizado com muita dedicação e envolvimento, de forma que me sinto gratificado com o fato de que os objetivos traçados, nunca demasiadamente ambiciosos, foram alcançados.

Appendix A

Modeling and Simulation of HENs

The simulation of Heat Exchanger Networks involves the simultaneous solution of the equations that represent the models and their components, such as the thermal equipments, mixers and stream splitters. These models are composed by governing equations that describe the mass and energy balances, and the basic design equation. The type and complexity of the model of each heat exchanger significantly affect the efforts required for HEN simulation, with great influence on time required and quality of results. The focus is on the development of a general heat exchanger model that simplifies the simulations. The main topics covered by this Appendix are listed below:

(i) Static Modeling;

(ii) Dynamic Modeling;

(iii) Static Model for Disturbance Propagation and Control;

(iv) State Space and Transfer Function Models.

A.1 Static Modeling

A.1.1 Energy Balance and Design Equation

In the model described here, the energy balances are performed for steady-state operation with the main hypothesis of constant physical properties, and non occurrence of phase change. The design equation relates the heat load (Q) with the heat transfer area (A). Assuming the ideal countercurrent flow, the temperature driving force correspond the log mean temperature difference (ΔT_{ml}). The global heat transfer coefficient (U) is related to the thermal resistances between the fluids inside the equipment. Considering small wall thickness it is possible to neglect the wall resistance $(R_{wall} \approx 0)$. The energy balance and the design equation for the hypothesis assumed are represented by the following equations:

(i) Energy Balance for the Heat Flow:

$$Q = \dot{m}_h Cp_h \left(T_h^{in} - T_h^{out}\right) = w_h \left(T_h^{in} - T_h^{out}\right) \quad \text{(A.1)}$$

(ii) Energy Balance for the Cold Flow:

$$Q = \dot{m}_c Cp_c \left(T_c^{out} - T_c^{in}\right) = w_c \left(T_c^{out} - T_c^{in}\right) \quad \text{(A.2)}$$

(iii) Design Equation:

$$Q = UA\Delta T_{ml} \quad \text{(A.3)}$$

(iv) The Temperature Driving Force (ideal countercurrent flow):

$$\Delta T_{ml} = \begin{cases} \dfrac{\left(T_h^{in} - T_c^{out}\right) - \left(T_h^{out} - T_c^{in}\right)}{\ln\left(\left(T_h^{in} - T_c^{out}\right)/\left(T_h^{out} - T_c^{in}\right)\right)} & when\ w_h \neq w_c \\ \left(T_h^{in} - T_c^{out}\right) = \left(T_h^{out} - T_c^{in}\right) & when\ w_h = w_c \end{cases} \quad \text{(A.4)}$$

(v) Global heat transfer Coefficient:

$$\frac{1}{U} = \sum R = \frac{1}{h_h} + \frac{1}{h_c} \quad \text{(A.5)}$$

A.1.2 Heat Transfer Coefficients

The heat transfer coefficients depend on, (i) fluid properties: such as, heat capacity (Cp); viscosity (μ); thermal conductivity (k); density (ρ); (ii) and flow properties: pipe diameter (D), and average flow velocity (v). A dimensional analysis shows the relation between the variables:

$$\frac{h}{Dk} = f\left(\frac{\rho v D}{\mu}, \frac{Cp\mu}{k}\right) \quad \text{(A.6)}$$

$$Nu = f(Re, Pr) \quad \text{(A.7)}$$

And the dimensionless groups involved are: (i) the *Reynolds Number* (Re), which represents the ratio of convective to molecular transport; (ii) the *Prandtl Number* (Pr), the ratio of momentum to heat transfer; and the *Nusselt Number* (Nu). Most of the correlations will thus take the form:

$$Nu = aRe^{b}Pr^{c} \tag{A.8}$$

The choice of a proper correlation depends on the flow regime, on the geometry, and whether or not a phase change occurs. It is assumed a shell and tube heat exchanger, since it is the most common type of heat exchanger in industrial processes. For the turbulent flow through the tubes, it is used a common and particularly simple correlation useful for many applications. The Dittus–Boelter heat transfer correlation:

$$h_t = 0.023\frac{k_t}{D_t}Re_t^{0.8}Pr_t^{1/3} \tag{A.9}$$

For the flow inside the shell, it is used the correlation presented by Kern (1950). The uncertainty of this correlation is notorious, however, its simplicity makes it, still, one of the main correlation used to estimate the heat transfer coefficient (h_s) in the flow that not present phase change, where D_e is the equivalent shell diameter.

$$h_s = 0.36\frac{k_s}{D_e}Re_s^{0.55}Pr_s^{1/3} \tag{A.10}$$

The use of the correlations requires the estimation, or arbitrary fixation, of some parameters. The external data, provided by the user are: (i) the tube outside diameter $(D_t)\{3/4\ in\}$; (ii) the heat transfer area (A); (iii) the tube wall thickness $(\delta_t)\{0\ in\}$; (iv) the number of baffles $(N_b)\{10\}$; (v) the ration between the tubes length and the shell diameter $(\varepsilon = L/D_s)\{8\}$; (vi) the ration between the tube pitch (Pt) and the tube diameter $(Pt/D_t)\{1.25\}$; (vii) the fluid on tube and shell side {cold flow in the shell side}; and (viii) the tube layout (square or {equilateral triangle}). The default values, indicated in brackets, correspond to typical values or design recommendations. The pressure drop is neglected, and the recommend flow velocity range is not verified.

For the flow in the tube side, we have:

(i) *Number of tubes* (N_t), *considered the near integer:*

$$N_t = round\left\{\frac{A}{\pi D_t L}\right\} = round\left\{\frac{A}{\pi D_t D_s \varepsilon}\right\} \tag{A.11}$$

where D_s is the shell diameter estimated by the equation (A.12) where $\alpha = 4$ for uare layout, and $2\sqrt{3}$ for triangular layout.

$$D_s = \sqrt[3]{\frac{\alpha A Pt^2}{\pi^2 \varepsilon D_t}} \tag{A.12}$$

(ii) *The tube length* (L):

$$L = \frac{A}{\pi D_t N_t} \tag{A.13}$$

(iii) *The tube flow area* (A_t):

$$A_t = \frac{\pi N_t (D_t - 2\delta_t)^2}{4} \tag{A.14}$$

(iv) *The average flow velocity* (v_t):

$$v_t = \frac{\dot{m}_t}{\rho_t A_t} = \frac{4\dot{m}_t}{\pi \rho_t N_t (D_t - 2\delta_t)^2} \tag{A.15}$$

(v) *The Reynolds number for the flow through the tubes*(Re_t):

$$Re_t = \frac{(D_t - 2\delta_t)\rho_t v_t}{\mu_t} \tag{A.16}$$

For the flow in the shell side:

(i) *Equivalent shell diameter* (D_e) :

$$D_e = \frac{4\left(\alpha_e (Pt)^2 - \frac{\pi D_t^2}{4}\right)}{\pi D_t} \tag{A.17}$$

with $\alpha_e = 1$ for square layout and $\sqrt{3/2}$ for triangular layout.

(ii) *Baffle spacing* (B_b):

$$B_b = \frac{L}{N_b - 1} \tag{A.18}$$

(iii) *The shell flow area* (A_s):

$$A_s = \frac{D_s (Pt - D_t) B_b}{Pt} \tag{A.19}$$

(iv) *The average flow velocity-shell side* (v_s):

$$v_s = \frac{\dot{m}_s}{\rho_s A_s} = \frac{\dot{m}_s Pt}{\rho_s \, D_s (Pt - D_t) B_b} \tag{A.20}$$

(v) *The Reynolds number for the flow through the shell* (Re_s):

$$Re_s = \frac{D_s \rho_s v_s}{\mu_s} \tag{A.21}$$

It is also possible the specification of the heat transfer coefficients. In that case, it is necessary to correct the heat transfer coefficient when the reference stream is splitted through the following equation:

$$h_c = h_{ref}\left(\frac{\dot{m}_c}{\dot{m}_{ref}}\right)^{0.8} \tag{A.22}$$

where h_{ref} is the specified value to the heat coefiicent that correspond to the mass flow $\dot{m}_{ref}$ of the stream that feed the process. The coeficinet h_c is the corrected coeficient use trough d in the fraction of the original stream with a flow $\dot{m}_c$.

A.1.3 Heat Exchanger

The operational variables presented in the modeling equations are identified in Figure A.1. Using the equations (A.1), (A.2), and (A.3) it is possible to explicit the outlet temperatures of the fluids in terms of known process parameters (Model HE01).

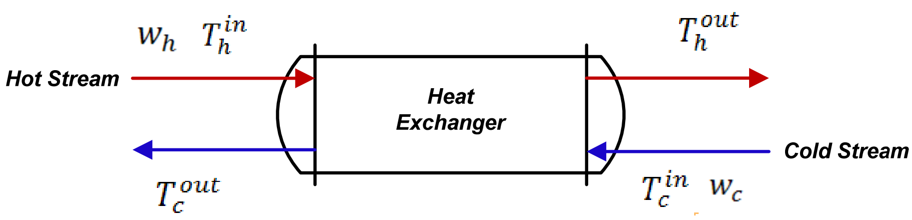


Figure A.1: General structure of a heat exchanger.

Model HE01: Model for Heat Exchanger Simulation.

Outlet Temperatures:

$$\begin{bmatrix} T_h^{out} \\ T_c^{out} \end{bmatrix} = \frac{1}{R_h - a}\begin{bmatrix} R_h - 1 & 1 - a \\ R_h(1-a) & a(R_h - 1) \end{bmatrix}\begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{A.23}$$

Ratio between heat capacity flow rates:

$$R_h \equiv \frac{w_h}{w_c} = \frac{T_c^{out} - T_c^{in}}{T_h^{in} - T_h^{out}} \tag{A.24}$$

Ratio between terminal temperature differences:

$$a \equiv \frac{T_h^{in} - T_c^{out}}{T_h^{out} - T_c^{in}} = exp\left(\frac{UA}{w_h}(1 - R_h)\right) \tag{A.24}$$

If we explicit the equation (A.23) in terms of inlet and outlet temperatures we have:

$$\begin{bmatrix} T_h^{out} \\ T_c^{out} \end{bmatrix} = \begin{bmatrix} 1 - P_h & P_h \\ P_c & 1 - P_c \end{bmatrix}\begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{A.25}$$

Where P_h and P_c are the thermal effectiveness defined by the equations:

$$P_h = \frac{T_h^{in} - T_h^{out}}{T_h^{in} - T_c^{in}} \quad and \quad P_c = \frac{T_c^{out} - T_c^{in}}{T_h^{in} - T_c^{in}} \tag{A.26}$$

A.1.4 Heat Exchanger with Bypass

For a heat exchanger with bypass option sketched in Figure A.2, with bypass fractions u_h and u_c for the hot and the cold side respectively, the modeling equations can be readily derived with we apply the Model HE01 to the inner part of the general structure and a mixer energy balance resulting in the Model HE02. In that case, if the heat transfer coefficients are given, the global heat transfer coefficient must be corrected according bypass fractions.

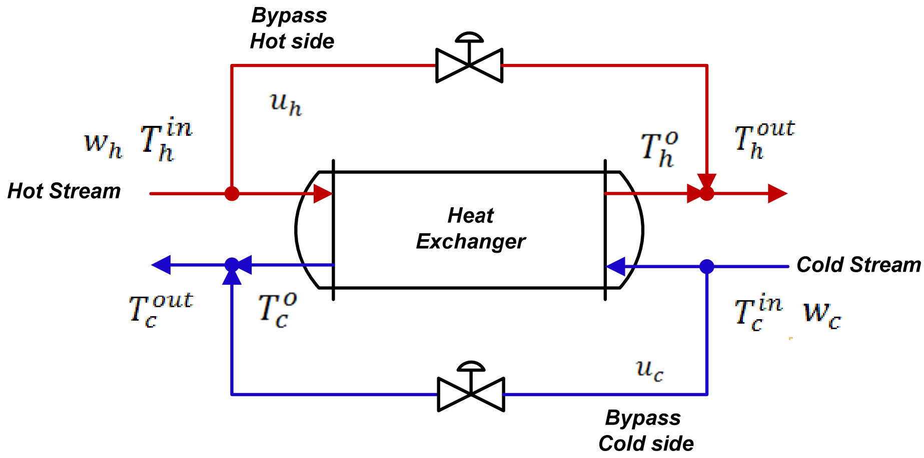


Figure A.2: General structure of a heat exchanger with bypasses.

Model HE02: Heat Exchanger with Bypasses.

Mixer Energy Balance:

$$\begin{bmatrix} T_h^{out} \\ T_c^{out} \end{bmatrix} = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{A.27}$$

Inner Heat Exchanger Structure:

$$\begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} = \frac{1}{(R_h' - a')} \begin{bmatrix} R_h' - 1 & 1 - a' \\ R_h'(1-a') & a'(R_h' - 1) \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \tag{A.28}$$

Ratio between effective heat capacity flow rates:

$$R_h' \equiv \frac{(1-u_h)w_h}{(1-u_c)w_c} = \frac{T_c^o - T_c^{in}}{T_h^{in} - T_h^o} \tag{A.29}$$

Ratio between terminal temperature differences:

$$a' \equiv \frac{T_h^{in} - T_c^o}{T_h^o - T_c^{in}} = \exp\left(\frac{U'A}{(1-u_h)w_h} (1 - R_h') \right) \tag{A.30}$$

Corrected Global Heat Transfer Coefficient:

$$\frac{1}{U'} = \frac{1}{h_h(1-u_h)^{0.8}} + \frac{1}{h_c(1-u_c)^{0.8}} \tag{A.31}$$

A.1.5 Heaters and Coolers

The heaters and coolers complete the thermal equipment of a HEN. In this case, the objectives during the simulation are different from the heat exchangers. These utility units are commonly placed to heat or cool streams just before leaving the HEN. Therefore, the utility loads must be estimated to ensure that the stream achieves its target. This utility load is estimated from the process stream requirement, and the mass flow rate according the required heat load and operational constrain on the utility outlet temperature.

The coolers are modeled through the following equations:

(i) *Cold Utility Load*:

$$Q_{cu} = \dot{m}_h Cp_h\left(T_h^{in} - T_h^{out}\right) = \dot{m}_h Cp_h\left(T_h^{in} - T_h^{target}\right) \quad \text{(A.32)}$$

(ii) *Cold Utility flowrate*:

$$\dot{m}_{cu} = \frac{Q_{cu}}{Cp_{cu}\left(T_{cu}^{out} - T_{cu}^{in}\right)} \quad \text{(A.33)}$$

(iii) *Heat transfer Area:*

$$A_{cu} = \left(\frac{1}{h_h} + \frac{1}{h_{cu}}\right)\frac{Q_{cu}\ ln\left(\left(T_h^{in} - T_{cu}^{out}\right)/\left(T_h^{out} - T_{cu}^{in}\right)\right)}{\left(T_h^{in} - T_{cu}^{out}\right) - \left(T_h^{out} - T_{cu}^{in}\right)} \quad \text{(A.34)}$$

Where

$$T_{cu}^{out} = min\left\{T_{cu}^{out,max}, T_h^{in} - \Delta T_{min}\right\} \quad \text{(A.35)}$$

And the Heaters:

(i) *Hot Utility Load*:

$$Q_{hu} = \dot{m}_c Cp_c\left(T_c^{out} - T_c^{in}\right) = \dot{m}_c Cp_c\left(T_c^{target} - T_c^{in}\right) \quad \text{(A.36)}$$

(ii) *Hot Utility flowrate*:

$$\dot{m}_{hu} = \frac{Q_{hu}}{Cp_{hu}\left(T_{hu}^{in} - T_{hu}^{out}\right)}\ , or\ \ \dot{m}_{hu} = \frac{Q_{hu}}{\Delta h_{vap}} \quad \text{(A.37)}$$

(iii) Heat transfer Area:

$$A_{hu} = \left(\frac{1}{h_{hu}} + \frac{1}{h_c}\right)\frac{Q_{hu}\ ln\left(\left(T_{hu}^{in} - T_c^{out}\right)/\left(T_{hu}^{out} - T_c^{in}\right)\right)}{\left(T_{hu}^{in} - T_c^{out}\right) - \left(T_{hu}^{out} - T_c^{in}\right)} \quad \text{(A.38)}$$

where

$$T_{hu}^{out} = max\left\{T_{hu}^{out,max}, T_c^{in} + \Delta T_{min}\right\} \quad \text{(A.39)}$$

A.1.6 Static Simulator

The static simulator for Heat Exchangers Networks was developed in Simulink 3.0. and Matlab. The main blocks that compose the simulation environment are described in this section, and a general overview is presented in Figure A.3.

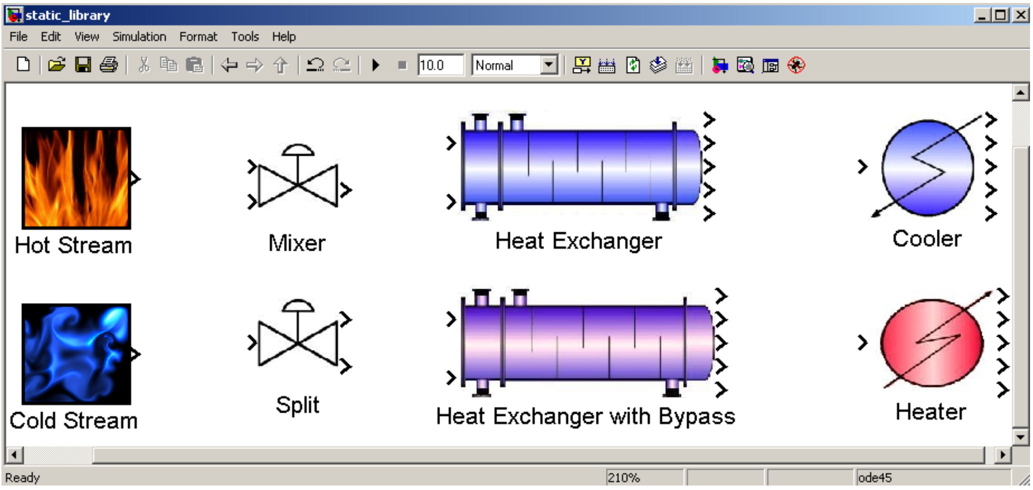


Figure A.3: Static Library with all blocks.

Process Streams

The process streams are structured with seven informations, that can be configured as can be seen in Figure A.4. The heat transfer coefficient corresponds to the stream mass flow, and its value is corrected in splits and heat exchangers with bypasses. It is also possible to estimate the heat transfer coefficient according to the section A.1.2, this option is informed in the heat exchanger blocks and it requires the thermo physical properties of fluid. When this option is selected the heat transfer coefficient informed is not considered.

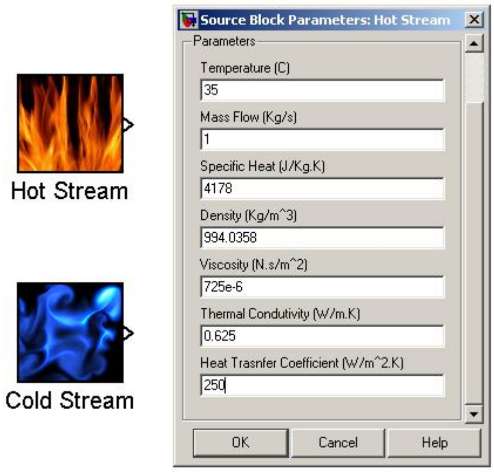
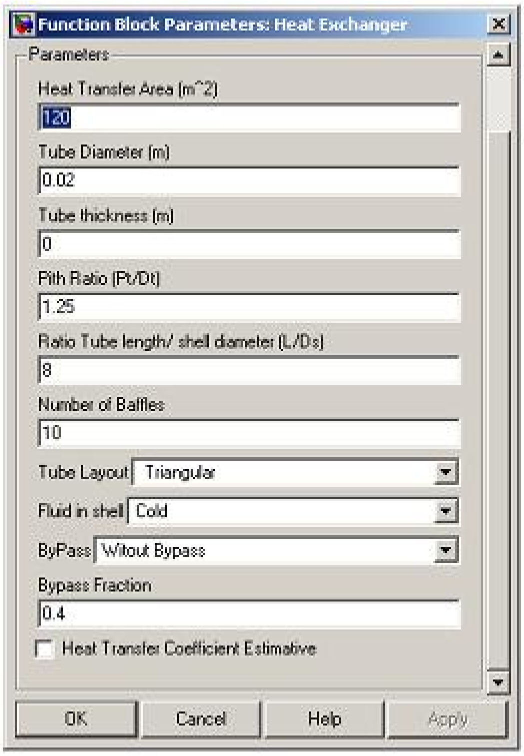


Figure A.4: Configuration window of the block stream.

Heat Exchangers

There are two blocks to simulate heat exchangers, heat exchanger with or without bypasses. It must be inserted the minimum equipment information. The tube layout, the fluid in shell and the presence of bypass present discrete options that must be selected using the popup menu. If the heat transfer coefficient must be estimated using the geometry and the fluid properties, defined in the stream block, the correspondent check box must be selected. The block also provides the steady-state gain matrices for disturbances in the inlet temperatures, the inlet flow and the bypass fraction. The Figure A.5 shows a sample of the block connections, and the configuration window.



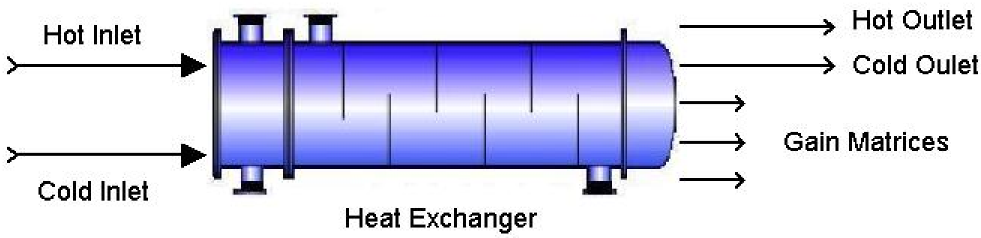


Figure A.5: Heat Exchanger block with its respective configuration window.

Utility Exchangers

The utility exchanger blocks are developed according to the modeling described in the section A.1.5. The block is feed with one process stream, and it is configured with the target of the process stream, and the utility data, informed through the block configuration window. The block outputs are the process stream, heated or cooled, and the heat loads, heat transfer area, utility outlet temperature and flow rate as presented in Figure A.6.

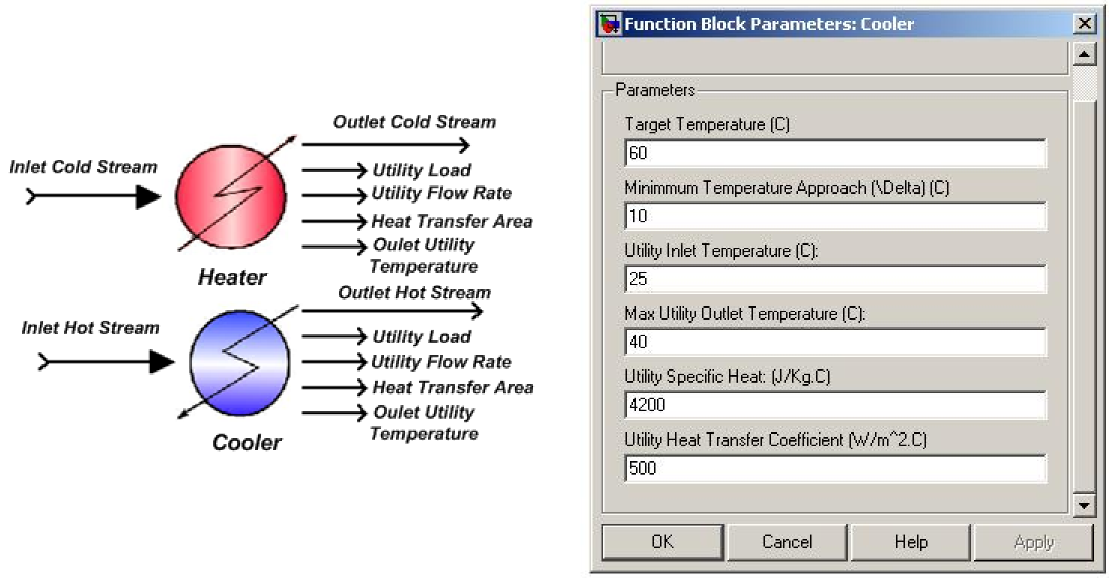


Figure A.6: Utility exchanger blocks, and configuration window for cooler block.

Mixers and Splitters

For the connections between streams in a HEN it is necessary the blocks mixer and splitters. For the mixer it is necessary only the energy balance to estimate the outlet temperature, and for the split it is necessary to provide the split fraction and only a mass balance is necessary. The internal routines correct the heat transfer coefficient according the mass flow of the streams involved in the process.

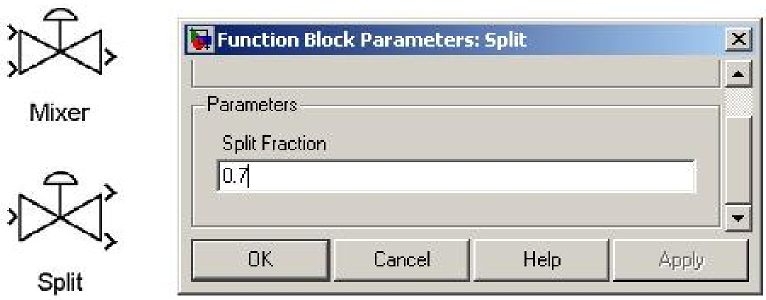


Figure A.7: Mixer and Split blocks, and configuration window for the split block.

Heat Exchanger Network Simulation

Using the static library and the Simulink environment it is possible to connect blocks and create the flowsheet with the HEN structure. A simple example is used to illustrate the potentiality of the developed tool, depicted in Figure A.8. The models are oriented to HEN control and optimization facilities, where is allowed the use of Matlab potential.

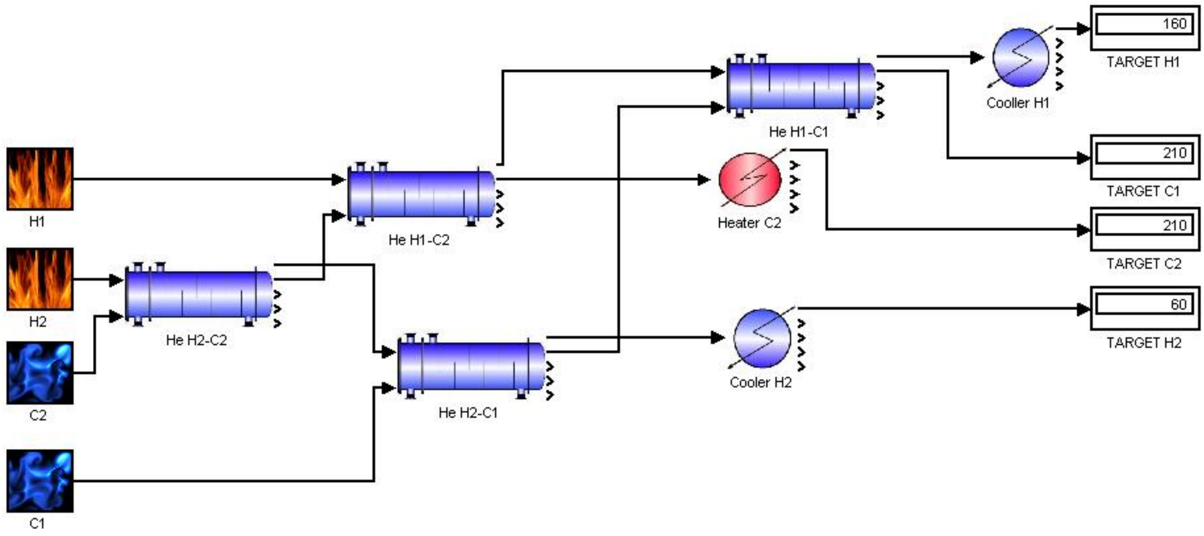


Figure A.8: Example of a HEN Simulation.

A.2 Dynamic Modeling

The complexity of the heat exchanger model greatly influence the time required and quality of results from a HEN simulation. The model must be simple, but with good agreement with steady-state behavior of ideal countercurrent heat exchangers.

The lumped compartment or "multicell" model of a heat exchanger is depicted in Figure A.9. The model is based on the hypothesis that a heat exchanger dynamic behavior can be described by a series of N ideal mixing tank. In addition to ideal mixing tank assumptions, it is assumed: (i) constant densities; (ii) constant specific heat capacities; (iii) constant and flow independent heat transfer coefficient; (iv) no phase changes; (v) pressure drop neglected; and that exchanger area A and volume V are equally distributed over the N cells.

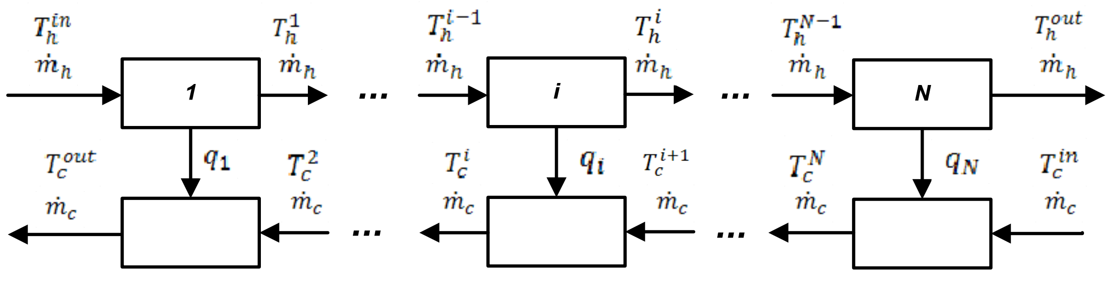


Figure A.9: Sketch of mixing tank model.

The model for each stage can be described by the following equations:

$$\rho_h V_h^i Cp_h \frac{dT_h^i}{dt} = \dot{m}_h Cp_h \left(T_h^{i-1} - T_h^i\right) - UA^i \Delta T_{ef}^i \tag{A.40}$$

$$\rho_c V_c^i Cp_c \frac{dT_c^i}{dt} = \dot{m}_c Cp_c \left(T_c^{i+1} - T_c^i\right) + UA^i \Delta T_{ef}^i \tag{A.41}$$

The heat transfer area of each cell ($A^i = A/N$) is determined by the total area (A) and the number of tanks (N). The volume of hot and cold fluid in each cell is determined by the total volume in the tube side and the hot side and the total number of cells. Supposing the hot fluid flowing through the shell and the cold fluid flowing through the tubes, we have:

$$V_h^i = \frac{V_h}{N} = \frac{\pi N_t L(D_t - 2\delta_t)^2}{4N} \tag{A.42}$$

$$V_c^i = \frac{V_c}{N} = \frac{\pi D_s^2 L - \pi N_t L D_t^2}{4N} \tag{A.43}$$

The effective temperature driving force for each cell can be represented using different alternatives. The first alternative underestimates the transferred heat at steady-state since the driving forces are less than for ideal countercurrent flow, the arithmetic mean compensates for the underestimation and the logarithmic mean give perfect accordance at steady-state. However this alternative may give serious problem in a dynamic simulation, because it is not defined when the temperature differences are equal, and for example, in a dynamic simulation for an inlet temperature can result in crossover in the heat exchanger until steady-state be reached. The Patterson approximation (Patterson, 1984) and Chen approximation (Chen, 1987) are good approximations of LMTD and can be used to avoid discontinuity when the temperature differences are equal but both give the same problems as LMTD when crossover occurs, since they involve geometric mean, thus they are not suited for dynamic simulations.

Pure Mixing Tank Model:

$$\Delta T_{ef}^i = T_h^i - T_c^i \tag{A.44}$$

Arithmetic mean Temperature difference (AMTD):

$$\Delta T_{ef}^i = \frac{\left(T_h^{i-1} - T_c^i\right) + \left(T_h^i - T_c^{i+1}\right)}{2} \tag{A.45}$$

Logarithmic mean Temperature difference (LMTD):

$$\Delta T_{ef}^i = \frac{\left(T_h^{i-1} - T_c^i\right) - \left(T_h^i - T_c^{i+1}\right)}{ln\left(\left(T_h^{i-1} - T_c^i\right)/\left(T_h^i - T_c^{i+1}\right)\right)} \tag{A.46}$$

LMTD Patterson (1982) Approximation:

$$\Delta T_{ef}^i = \frac{1}{3}\frac{\left(T_h^{i-1} - T_c^i\right) + \left(T_h^i - T_c^{i+1}\right)}{2} + \frac{2}{3}\sqrt{\left(T_h^{i-1} - T_c^i\right)\left(T_h^i - T_c^{i+1}\right)} \tag{A.47}$$

LMTD Chen (1987) Approximation:

$$\Delta T_{ef}^i = \left[\frac{\left(T_h^{i-1} - T_c^i\right) + \left(T_h^i - T_c^{i+1}\right)}{2}\left(T_h^{i-1} - T_c^i\right)\left(T_h^i - T_c^{i+1}\right)\right]^{\frac{1}{3}} \tag{A.48}$$

It is also possible taking into account the influence of the wall in the dynamic behavior through a simplified model. For this particular case, there is a need of adding one more equation to describe the behavior of each stage. It is considered constant properties of the wall, axial conduction neglected, and a small wall thickness. Therefore we have:

$$\rho_w V_w^i Cp_w \frac{dT_w^i}{dt} = \frac{A_h}{N} h_h \Delta T_{ef,wh}^i - \frac{A_c}{N} h_c \Delta T_{ef,wc}^i \tag{A.49}$$

$$V_w^i = \frac{V_w}{N} = \frac{\pi N_t L (D_t^2 - (D_t - 2\delta_t)^2)}{4N} \tag{A.50}$$

The effective temperature difference between the hot fluid and the wall ($\Delta T_{ef,wh}^i$), and between the wall and the cold fluid ($\Delta T_{ef,wc}^i$), are estimated according the options expressed in equations (A.44) to (A.48).

A.2.1 Dynamic Simulator

In the dynamic version of the simulator, the structure of the streams is similar to the stationary simulator, but the configuration window of the stream block allows the specification the dynamic characteristics for a step perturbation in the inlet temperatures and flow rates. The heat exchangers requires besides the same information for static simulation, the number of cells, and the method for effective temperature difference (all five possibilities shown are permissible), and a check box to consider the influence of the wall.

A.3 Static Model for Disturbance Propagation and Control

Unit-based Model

The complete static model for disturbance propagation that characterizes the system behavior under control can be described by the following equation

$$\delta T^{out} = G_u \delta u + G_d^t \, \delta T^{in} + G_d^w \, \delta w \tag{A.50}$$

where the vectors are described below:

$$\delta T^{out} = [\delta T_h^{out} \quad \delta T_c^{out}]^T \tag{A.51}$$

$$\delta u = [\delta u_h \quad \delta u_c]^T \tag{A.52}$$

$$\delta T^{in} = [\delta T_h^{in} \quad \delta T_c^{in}]^T \tag{A.53}$$

$$\delta w = [\delta w_h \quad \delta w_c]^T \tag{A.54}$$

To obtain the matrices (G_u, G_d^t, G_d^w), the first step consists in the linearization of the model HE01 (without bypasses for instance). Using Taylor series expansion, neglecting high-order differentiation terms result in the model for disturbance propagation HEDP.

Model HEDP: Model for Disturbance Propagation (without bypass).

$$\begin{bmatrix}\delta T_h^{out}\\ \delta T_c^{out}\end{bmatrix} = \begin{bmatrix}1-P_h & P_h\\ P_c & 1-P_c\end{bmatrix}\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + \left(T_h^{in}-T_c^{in}\right)\begin{bmatrix}A_w & B_w\\ C_w & D_w\end{bmatrix}\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} \quad (A.55)$$

$$A_w = -\frac{(R_h-1)aNTU_h + R_h(a-1)}{w_h(R_h-a)^2} \quad (A.56)$$

$$B_w = \frac{(R_h-1)aNTU_c + R_h(a-1)}{w_c(R_h-a)^2} \quad (A.57)$$

$$C_w = \frac{(R_h-1)NTU_h + (a-1)}{w_h(R_h-a)^2}(aR_h) \quad (A.58)$$

$$D_w = -\frac{(R_h-1)NTU_c + (a-1)}{w_c(R_h-a)^2}(aR_h) \quad (A.59)$$

$$NTU_h = \frac{UA}{w_h}\ ;\ NTU_c = \frac{UA}{w_c} \quad (A.60)$$

Now considering the heat exchangers with bypass on the cold and hot side, the model HEDP can be applied to the inner part of the system, i.e. between the inlet and the outlet of the heat exchanger where w_h^e and w_c^e consist in the heat capacity flow rate that effectively enters the heat exchanger, and T_h^o and T_c^o consist in the outlet temperatures for the heat exchanger. The "inner" model is described as follows:

$$\begin{bmatrix}\delta T_h^{o}\\ \delta T_c^{o}\end{bmatrix} = \begin{bmatrix}1-P_h' & P_h'\\ P_c' & 1-P_c'\end{bmatrix}\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + \left(T_h^{in}-T_c^{in}\right)\begin{bmatrix}A_w' & B_w'\\ C_w' & D_w'\end{bmatrix}\begin{bmatrix}\delta w_h^e\\ \delta w_c^e\end{bmatrix} \quad (A.61)$$

$$A_w' = -\frac{(R_h'-1)a'NTU_h' + R_h'(a'-1)}{w_h(1-u_h)(R_h'-a')^2} \quad (A.62)$$

$$B_w' = \frac{(R_h'-1)a'NTU_c' + R_h'(a'-1)}{w_c(1-u_c)(R_h'-a')^2} \quad (A.63)$$

$$C_w' = \frac{(R_h'-1)NTU_h' + (a'-1)}{w_h(1-u_h)(R_h'-a')^2}(a'R_h') \quad (A.64)$$

$$D_w' = -\frac{(R_h'-1)NTU_c' + (a'-1)}{w_c(1-u_c)(R_h'-a')^2}(a'R_h') \quad (A.65)$$

$$P_h' = \frac{T_h^{in} - T_h^{out\prime}}{T_h^{in} - T_c^{in}}\ ;\ P_c' = \frac{T_c^{out\prime} - T_c^{in}}{T_h^{in} - T_c^{in}} \quad (A.66)$$

$$NTU_h' = \frac{U'A}{w_h(1-u_h)}\ ;\ NTU_c' = \frac{U'A}{w_c(1-u_c)} \quad (A.67)$$

The vectors $[\delta w_h^e \quad \delta w_c^e]^T$ and $[\delta T_h^o \quad \delta T_c^o]^T$ in the preceding model should be converted to $[\delta w_h \quad \delta w_c]^T$ and $[\delta T_h^{out} \quad \delta T_c^{out}]^T$, respectively. Note that the heat capacity flow rate that effectively enters in the heat exchanger can be expressed by the following equation:

$$\begin{bmatrix} w_h^e \\ w_c^e \end{bmatrix} = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} w_h \\ w_h \end{bmatrix} \tag{A.68}$$

Its differentiation gives

$$\begin{bmatrix} \delta w_h^e \\ \delta w_c^e \end{bmatrix} = \begin{bmatrix} -w_h & 0 \\ 0 & -w_c \end{bmatrix} \begin{bmatrix} \delta u_h \\ \delta u_c \end{bmatrix} + \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} \delta w_h \\ \delta w_h \end{bmatrix} \tag{A.69}$$

And the differentiation of the heat balance in the mixer (A.27) gives

$$\begin{aligned} \begin{bmatrix} \delta T_h^{out} \\ \delta T_c^{out} \end{bmatrix} &= \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} \delta T_h^o \\ \delta T_c^o \end{bmatrix} + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix} \begin{bmatrix} \delta T_h^{in} \\ \delta T_c^{in} \end{bmatrix} \\ &+ \begin{bmatrix} T_h^{in} - T_h^o & 0 \\ 0 & T_c^{in} - T_c^o \end{bmatrix} \begin{bmatrix} \delta u_h \\ \delta u_c \end{bmatrix} \end{aligned} \tag{A.70}$$

From equation (A.27) we can derive

$$\begin{bmatrix} T_h^{in} - T_h^o & 0 \\ 0 & T_c^{in} - T_c^o \end{bmatrix} = \begin{bmatrix} \dfrac{T_h^{in} - T_h^{out}}{1-u_h} & 0 \\ 0 & \dfrac{T_c^{in} - T_c^{out}}{1-u_c} \end{bmatrix} \tag{A.71}$$

Substituting the equation (A.69) into the model (A.61), and substituting the resulting expression into the equation (A.70), we can obtain the following model:

Model HEDP&C: Model for disturbance propagation and control.

$$\begin{bmatrix} \delta T_h^{out} \\ \delta T_c^{out} \end{bmatrix} = G_d^t \begin{bmatrix} \delta T_h^{in} \\ \delta T_c^{in} \end{bmatrix} + G_d^w \begin{bmatrix} \delta w_h \\ \delta w_h \end{bmatrix} + G_u \begin{bmatrix} \delta u_h \\ \delta u_c \end{bmatrix} \tag{A.72}$$

$$G_d^t = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} 1-P_h' & P_h' \\ P_c' & 1-P_c' \end{bmatrix} + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix} \tag{A.73}$$

$$G_d^w = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \left(T_h^{in} - T_c^{in}\right) \begin{bmatrix} A_w' & B_w' \\ C_w' & D_w' \end{bmatrix} \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \tag{A.74}$$

$$G_u = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \left(T_h^{in} - T_c^{in}\right) \begin{bmatrix} A'_w & B'_w \\ C'_w & D'_w \end{bmatrix} \begin{bmatrix} -w_h & 0 \\ 0 & -w_c \end{bmatrix} + \begin{bmatrix} \dfrac{T_h^{in} - T_h^{out}}{1-u_h} & 0 \\ 0 & \dfrac{T_c^{in} - T_c^{out}}{1-u_c} \end{bmatrix} \tag{A.75}$$

HEN Disturbance Propagation Model and Control

The model HEDP&C in equation (A.50) is applicable to each heat exchanger in a HEN. The model for the ith heat exchanger, named E_i, in a network can be rewritten as

$$\delta T_{E_i}^{out} = G_{u,E_i} \delta u_{E_i} + G_{d,E_i}^{t}\, \delta T_{E_i}^{in} + G_{d,E_i}^{w}\, \delta w_{E_i} \tag{A.76}$$

If a HEN contains N_e heat exchangers, a system model can be obtained directly by lumping all unit models in the sequence of exchanger numbers.

$$\delta T^{*out} = G_{u,E}^{*} \delta u^{*} + G_{d,E}^{*t}\, \delta T^{*in} + G_{d,E}^{*w}\, \delta w^{*} \tag{A.77}$$

where

$$\delta T^{*out} = \left[\left(\delta T_{E_1}^{out}\right)^T \left(\delta T_{E_2}^{out}\right)^T \ldots \left(\delta T_{E_{N_e}}^{out}\right)^T \right]^T \tag{A.78}$$

$$\delta T^{*in} = \left[\left(\delta T_{E_1}^{in}\right)^T \left(\delta T_{E_2}^{in}\right)^T \ldots \left(\delta T_{E_{N_e}}^{i}\right)^T \right]^T \tag{A.79}$$

$$\delta w^{*} = \left[\left(\, \delta w_{E_1}\right)^T \left(\delta w_{E_2}\right)^T \ldots \left(\delta w_{E_{N_e}}\right)^T \right]^T \tag{A.80}$$

$$\delta u^{*} = \left[\left(\, \delta u_{E_1}\right)^T \left(\delta u_{E_2}\right)^T \ldots \left(\delta u_{E_{N_e}}\right)^T \right]^T \tag{A.81}$$

$$G_{u,E}^{*} = diag\left\{ G_{u,E_1}, G_{u,E_2}, \ldots, G_{u,E_{N_e}} \right\} \tag{A.82}$$

$$G_{d,E}^{*t} = diag\left\{ G_{d,E_1}^{t}, G_{d,E_2}^{t}, \ldots, G_{d,E_{N_e}}^{t} \right\} \tag{A.83}$$

$$G_{d,E}^{*w} = diag\left\{ G_{d,E_1}^{w}, G_{d,E_2}^{w}, \ldots, G_{d,E_{N_e}}^{w} \right\} \tag{A.84}$$

The dimension of vectors $\delta T^{*out}, \delta T^{*in}, \delta w^{*}$ and δu^{*} are all $2N_e \times 1$ and the matrices $G_{u,E}^{*}$, $G_{d,E}^{*t}$ and $G_{d,E}^{*w}$ are all $2N_e \times 2N_e$. Note that δT^{*out} and δT^{*in} contain a total of N_m intermediate temperatures. An intermediate temperature is that of a stream between two adjacent heat exchangers. The term, N_m can be evaluated as

$$N_m = 2N_e - N_s - N_{split} \tag{A.85}$$

Where N_s is the total number of streams; and N_{split} is the total number of branches after splitting. The temperature vectors can be organized according to the supply and target temperatures of the streams that are present in the HEN in the following manner.

$$\begin{aligned}\delta T^{in} &= \left[\delta T_{H1}^{s} \dots \delta T_{HN_h}^{s}\, \delta T_{C1}^{s} \dots \delta T_{CN_c}^{s}\ \delta T_{1}^{m} \dots \delta T_{N_m}^{m}\ \right]^T \\ &= [(\delta T^S)^T (\delta T^m)^T]^T\end{aligned} \tag{A.86}$$

$$\begin{aligned}\delta T^{out} &= \left[\delta T_{H1}^{T} \dots \delta T_{HN_h}^{T}\, \delta T_{C1}^{T} \dots \delta T_{CN_c}^{T}\ \delta T_{1}^{m} \dots \delta T_{N_m}^{m}\ \right]^T \\ &= [(\delta T^T)^T (\delta T^m)^T]^T\end{aligned} \tag{A.87}$$

The vector δw^* presents N_m redundant heat-capacity flow rates that should be eliminated. This reduces δw^* to $[(2N_e - N_m) \times 1]$. Correspondly,

$$G_u^* = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} = V_1 G_{u,E}^* V_4 \tag{A.88}$$

$$G_d^{*t} = \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} = V_1 G_{d,E}^{*t} V_2 \tag{A.89}$$

$$G_d^{*w} = \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} = V_1 G_{d,E}^{*w} V_3 \tag{A.90}$$

Where V_1 trough V_4 are the conversion matrices determined by a HEN structure and bypass location. Their derivations are presented in the succeeding section. The organized model is

$$\begin{bmatrix} \delta T^T \\ \delta T^m \end{bmatrix} = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} \delta u + \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} \begin{bmatrix} \delta T^S \\ \delta T^m \end{bmatrix} + \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} \delta w \tag{A.91}$$

The preceding model contains two equations, solving the latter to the intermediate temperatures and substituting in the former yields the following model:

$$\delta T^T = G_{u,hen} \delta u + G_{d,hen}^t \delta T^S + G_{d,hen}^w \delta w \tag{A.92}$$

where

$$G_{u,hen} = G_{u,1} + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{u,2} \tag{A.93}$$

$$G_{d,hen}^t = G_{d,11}^t + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{d,21}^t \tag{A.94}$$

$$G_{d,hen}^w = G_{d,1}^w + G_{d,12}^t \left(I - G_{d,22}^t\right)^{-1} G_{d,2}^w \tag{A.95}$$

In more detail, if the vectors of stream temperature and heat capacity flowrates are written based on classification of stream types, the model (A.92) can be written as

$$\begin{bmatrix}\delta T_h^T \\ \delta T_c^T\end{bmatrix} = G_{u,hen}\delta u + \begin{bmatrix}G_{d,hen,h}^t & G_{d,hen,c}^t\end{bmatrix}\begin{bmatrix}\delta T_h^S \\ \delta T_c^S\end{bmatrix} + \begin{bmatrix}G_{d,hen,h}^w & G_{d,hen,c}^w\end{bmatrix}\begin{bmatrix}\delta w_h \\ \delta w_c\end{bmatrix} \tag{A.96}$$

Where

$$\delta T_h^T = \left[\delta T_{h_1}^T \ \delta T_{h_2}^T \ldots \delta T_{h_{N_h}}^T\right]^T \tag{A.97}$$

$$\delta T_c^T = \left[\delta T_{c_1}^T \delta T_{c_2}^T \ldots \delta T_{c_{N_c}}^T\right]^T \tag{A.98}$$

$$\delta T_h^S = \left[\delta T_{h_1}^S \ \delta T_{h_2}^S \ldots \delta T_{h_{N_h}}^S\right]^T \tag{A.99}$$

$$\delta T_c^S = \left[\delta T_{c_1}^S \delta T_{c_2}^S \ldots \delta T_{c_{N_c}}^S\right]^T \tag{A.100}$$

$$\delta w_h = \left[\delta w_{h_1} \ \delta w_{h_2} \ldots \delta w_{h_{N_h}}\right]^T \tag{A.101}$$

$$\delta w_c = \left[\delta w_{c_1} \ \delta w_{c_2} \ldots \delta w_{c_{N_c}}\right]^T \tag{A.102}$$

$$\delta u = \left[\left(\delta u_{E_1}\right)^T \left(\delta u_{E_2}\right)^T \ldots \left(\delta u_{E_{N_e}}\right)^T\right]^T \tag{A.103}$$

Network Structural Representation

As stated in the proceeding section, conversion matrices V1 through V4 are structure dependent. According to the sequence of equipment considered, the original vector of output temperatures (δT^{*out}) will present a defined order involving the target temperatures (δT^T) and the intermediate temperatures (δT^m).

$\underline{Derivation\,of}$ V_1. Each element of matrix V_1 has a value 0 or 1 relating the disordered vector δT^{*out} with the ordered vector δT^{out}. Fist, the matrix V_1 must have all elements set to 0. The first row of V_1 (i) that corresponds to the $\delta T_{h_1}^T$ relation, considering that this target is located in the k position in the disordered vector, set $V_1(i,k)$=1. It should be noted that in case of stream split, where the same temperature enters two or more heat exchangers, there will be more than one position that represent the same target. Then, in a more general way k consist in a vector of corresponding positions. The procedure must be repeated until the last row of δT^{out}.

$\underline{Derivation\,of}$ V_2. The matrix V_2 is generated analogously to the matrix V_1. Each element of V_2 has a value 0 or 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to $\delta T_{h_1}^S$relation, select the k positions that this input appears in the vector δT^{*in} and for each position, set $V_2(k,j)$=1. Repeat the procedure until the last column.

$\underline{Derivation\ of}\ V_3$. Each element of V_3 has a value between 0 and 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to δw_{h_1}relation, select the k positions that this input appears in the vector δw^* and for each position, substitute by the split fraction of the original stream flowrate, $V_3(k,j) = x_s$. Repeat the procedure until the last column.

$\underline{Derivation\ of}\ V_4$.. Each element of V_4 has a value 0 or 1. This matrix is determined by the bypass selection in a HEN, i.e. $\delta u = V_4 \delta u_{sel.}$. If is desirable a model with all possible candidates, this matrix must be an identity matrix. To derive V_4, first all elements must be set to zero. Select the first column (j) that corresponds the first selected manipulated input $\delta u_{sel.}(1)$, select the k position that this input appears in the vector δu, set $V_4(k,j) = 1$. Repeat the procedure until the last column.

A.4 State Space and Transfer Function Models

Stationary Solution

It is necessary to solve the linear system of equations formed by the stationary condition applied to the equations (A.40) and (A.41), resulting

$$0 = \dot{m}_h Cp_h \left(T_h^{i-1} - T_h^i\right) - UA^i \Delta T_{ef}^i \tag{A.104}$$

$$0 = \dot{m}_c Cp_c \left(T_h^{i+1} - T_c^i\right) + UA^i \Delta T_{ef}^i \tag{A.105}$$

Independent of the choice to represent the effective temperature driving force for each cell $\left(\Delta T_{ef}^i\right)$, the output temperature vector for each cell can be described by the input vector as follows

$$\begin{bmatrix} T_h^i \\ T_c^i \end{bmatrix} = \begin{bmatrix} 1 - P_h^i & P_h^i \\ P_c^i & 1 - P_c^i \end{bmatrix} \begin{bmatrix} T_h^{i-1} \\ T_c^{i+1} \end{bmatrix} \tag{A.106}$$

Where P_h^i and P_c^i are the thermal effectiveness of each cell. They are independent of temperatures; it is a function of number of transfer units, heat capacity flowrate and flow configuration, and the effective temperature difference.

$$P_h^i \equiv \frac{T_h^{i-1} - T_h^i}{T_h^{i-1} - T_c^{i+1}} \ ; \ P_c^i \equiv \frac{T_c^i - T_c^{i+1}}{T_h^{i-1} - T_c^{i+1}} \tag{A.107}$$

For instance consider that the function is known, the derivations are presented in the next topic. For the stationary solution it is necessary to solve the following linear system of equations:

$$\begin{aligned} & A\begin{bmatrix} T_h^1 & T_h^2 & \dots & T_h^{N-1} & T_h^N & T_c^1 & T_c^2 & \dots & T_c^{N-1} & T_c^N \end{bmatrix}^T \\ &= \begin{bmatrix} \left(1 - P_h^i\right) T_h^{in} & 0 & \dots & 0 & P_h^N T_c^{in} & P_c^1 T_h^{in} & 0 & \dots & 0 & \left(1 - P_c^i\right) T_c^{in} \end{bmatrix}^T \end{aligned} \tag{A.108}$$

Where the matrix A is defined:

$$A = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 & 0 & -P_c^1 & \dots & 0 & 0 \\ P_h^2 - 1 & 1 & 0 & 0 & 0 & 0 & 0 & -P_c^2 & 0 & 0 \\ \vdots & \ddots & \ddots & 0 & 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & P_h^{N-1} - 1 & 1 & 0 & 0 & 0 & 0 & 0 & -P_c^{N-1} \\ 0 & 0 & 0 & P_h^N - 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 & 1 & P_c^1 - 1 & 0 & 0 & 0 \\ -P_h^2 & 0 & 0 & 0 & 0 & 0 & 1 & P_c^2 - 1 & 0 & 0 \\ \vdots & \ddots & 0 & 0 & 0 & 0 & 0 & 1 & \ddots & 0 \\ 0 & 0 & -P_h^{N-1} & 0 & 0 & 0 & 0 & 0 & 1 & P_c^{N-1} - 1 \\ 0 & 0 & 0 & -P_h^N & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{(A.109)}$$

Defining the Number of Transfer Units (NTU) of each cell:

$$NTU_h^i \equiv \frac{UA^i}{w_h} \; ; \; NTU_c^i \equiv \frac{UA^i}{w_c} \quad \text{(A.110)}$$

$$a_i = \exp\left(NTU_h^i(1 - R_h)\right) \quad \text{(A.111)}$$

The thermal effectiveness (P) can be calculated by the following equations:

Pure Mixing Tank:

$$P_h^i = \frac{NTU_h^i}{1 + NTU_h^i + NTU_c^i}; \; P_c^i = \frac{NTU_c^i}{1 + NTU_h^i + NTU_c^i} \quad \text{(A.112)}$$

Arithmetic Mean Temperature

$$P_h^i = \frac{2NTU_h^i}{2 + NTU_h^i + NTU_c^i}; \; P_c^i = \frac{2NTU_c^i}{2 + NTU_h^i + NTU_c^i} \quad \text{(A.113)}$$

Logarithmic Mean Temperature

$$P_h^i = \frac{1 - a_i}{R_h - a_i}; \; P_c^i = \frac{R_h(1 - a_i)}{R_h - a_i} \quad \text{(A.114)}$$

Linearization

The linearization is performed over the following equations:

$$\frac{dT_h^i}{dt} = f = \frac{\dot{m}_h Cp_h}{\rho_h V_h^i Cp_h}\left(T_h^{i-1} - T_h^i\right) - \frac{UA^i}{\rho_h V_h^i Cp_h}\Delta T_{ef}^i \quad \text{(A.115)}$$

$$\frac{dT_c^i}{dt} = g = \frac{\dot{m}_c Cp_c}{\rho_c V_c^i Cp_c}\left(T_c^{i+1} - T_c^i\right) + \frac{UA^i}{\rho_c V_c^i Cp_c}\Delta T_{ef}^i \quad \text{(A.116)}$$

Lets explicit the state vector in order to avoiding confusion, and it must be clear that the real inputs of the system are $T_h^{in} = T_h^0$ and $T_c^{in} = T_c^{N+1}$. And we are considering the heat capacity flowrates as disturbances $w_h = \dot{m}_h Cp_h$ and $w_c = \dot{m}_c Cp_c$.

$$\delta T_h^{i,out} = [T_h^1 \quad \dots \quad T_h^N]^T$$

$$\delta T_c^{i,out} = [T_c^1 \quad \dots \quad T_c^N]^T$$

$$\frac{d}{dt}\begin{pmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{pmatrix} = \begin{bmatrix}\frac{\partial f}{\partial T_h^{i,out}} & \frac{\partial f}{\partial T_c^{i,out}}\\ \frac{\partial g}{\partial T_h^{i,out}} & \frac{\partial g}{\partial T_c^{i,out}}\end{bmatrix}\begin{bmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{bmatrix} + \begin{bmatrix}\frac{\partial f}{\partial T_h^{in}}\\ \frac{\partial g}{\partial T_c^{in}}\end{bmatrix}\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + \begin{bmatrix}\frac{\partial f}{\partial w_h}\\ \frac{\partial g}{\partial w_h}\end{bmatrix}\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} \quad (A.118)$$

$$\begin{bmatrix}\delta T_h^{out}\\ \delta T_c^{out}\end{bmatrix} = \begin{bmatrix}\delta T_h^{N}\\ \delta T_c^{1}\end{bmatrix} = \begin{bmatrix}0 & \dots & 1 & 0 & \dots & 0\\ 0 & \dots & 0 & 1 & \dots & 0\end{bmatrix}\begin{bmatrix}\delta T_h^1\\ \vdots\\ \delta T_h^N\\ \delta T_c^1\\ \vdots\\ \delta T_c^N\end{bmatrix} \quad (A.119)$$

In order to simplify the notation, the general state space model without bypass can be expressed as follow, and the matrices A to D can be recognized by comparison with the previous equation.

$$\frac{d}{dt}\begin{pmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{pmatrix} = \begin{bmatrix}A_1\\ A_2\end{bmatrix}\begin{bmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{bmatrix} + \begin{bmatrix}B_1^t\\ B_2^t\end{bmatrix}\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + \begin{bmatrix}B_1^w\\ B_2^w\end{bmatrix}\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} \quad (A.120)$$

$$\begin{bmatrix}\delta T_h^{out}\\ \delta T_c^{out}\end{bmatrix} = C\begin{bmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{bmatrix} + D^t\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + D^w\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} \quad (A.121)$$

The model described by the equations (A.120) and (A.121) can be used for dynamic disturbance propagation. It must be necessary to consider the manipulated inputs, for instance we consider the bypass as candidates. To derive the complete model, the previous model for dynamic disturbance propagation can be used with the substitution of w_h by w_h^e and w_c by w_c^e , i.e. the flowrates that really enters the exchanger. The states of the two models are the same. It should be noted that the output vectors correspond to the temperatures after the mixing. Using the equations (A.69) and (A.70) the general model can be described by:

$$\frac{d}{dt}\begin{pmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{pmatrix} = \begin{bmatrix}A_1\\ A_2\end{bmatrix}\begin{bmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{bmatrix} + \begin{bmatrix}B_1^t\\ B_2^t\end{bmatrix}\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + \begin{bmatrix}B_3^w\\ B_4^w\end{bmatrix}\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} + \begin{bmatrix}B_1^u\\ B_2^u\end{bmatrix}\begin{bmatrix}\delta u_h\\ \delta u_c\end{bmatrix} \quad (A.122)$$

$$\begin{bmatrix}\delta T_h^{out}\\ \delta T_c^{out}\end{bmatrix} = C_m\begin{bmatrix}\delta T_h^{i,out}\\ \delta T_c^{i,out}\end{bmatrix} + D_m^t\begin{bmatrix}\delta T_h^{in}\\ \delta T_c^{in}\end{bmatrix} + D_m^w\begin{bmatrix}\delta w_h\\ \delta w_c\end{bmatrix} + D_m^u\begin{bmatrix}\delta u_h\\ \delta u_c\end{bmatrix} \quad (A.123)$$

Where:

$$\begin{bmatrix} B_3^w \\ B_4^w \end{bmatrix} = \begin{bmatrix} B_1^w \\ B_2^w \end{bmatrix} \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix}; \quad \begin{bmatrix} B_1^u \\ B_2^u \end{bmatrix} = \begin{bmatrix} B_1^w \\ B_2^w \end{bmatrix} \begin{bmatrix} -w_h & 0 \\ 0 & -w_c \end{bmatrix} \tag{A.124}$$

$$C_m = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} C; \quad D_m^u = \begin{bmatrix} \dfrac{T_h^{in} - T_h^{out}}{1-u_h} & 0 \\ 0 & \dfrac{T_c^{in} - T_c^{out}}{1-u_c} \end{bmatrix} \tag{A.125}$$

$$D_m^t = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} D^t + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix}; \; D_m^w = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} D^w \tag{A.126}$$

Matrices Derivation

In the previous section, it was presented a general model without the discrimination of the matrices that constitute it. The matrices for states can be written as follows:

$$A_1 = \begin{bmatrix} a_h^1 & 0 & \dots & 0 & 0 & c_h^1 & d_h^1 & \dots & 0 & 0 \\ b_h^2 & a_h^2 & 0 & 0 & 0 & 0 & c_h^2 & d_h^2 & 0 & 0 \\ 0 & \ddots & \ddots & \vdots & \vdots & \vdots & 0 & \ddots & 0 \ddots & \vdots \\ \vdots & 0 & b_h^{N-1} & a_h^{N-1} & 0 & 0 & 0 & 0 & c_h^{N-1} & d_h^{N-1} \\ 0 & 0 & 0 & b_h^N & a_h^N & 0 & 0 & \dots & 0 & c_h^N \end{bmatrix} \tag{A.127}$$

$$A_2 = \begin{bmatrix} a_c^1 & 0 & \dots & 0 & 0 & c_c^1 & d_c^1 & \dots & 0 & 0 \\ b_c^2 & a_c^2 & 0 & 0 & 0 & 0 & c_h^2 & d_c^2 & 0 & 0 \\ 0 & \ddots & \ddots & \vdots & \vdots & \vdots & 0 & \ddots & 0 \ddots & \vdots \\ \vdots & 0 & b_c^{N-1} & a_c^{N-1} & 0 & 0 & 0 & 0 & c_c^{N-1} & d_c^{N-1} \\ 0 & 0 & 0 & b_c^N & a_c^N & 0 & 0 & \dots & 0 & c_c^N \end{bmatrix} \tag{A.128}$$

And the matrices for inputs disturbances:

$$B_1^t = \begin{bmatrix} b_h^1 & 0 \\ \vdots & \vdots \\ 0 & d_h^N \end{bmatrix}; \; B_2^t = \begin{bmatrix} b_c^1 & 0 \\ \vdots & \vdots \\ 0 & d_c^N \end{bmatrix} \tag{A.129}$$

$$B_1^w = \begin{bmatrix} \gamma_h^1 & 0 \\ \vdots & \vdots \\ \gamma_h^N & 0 \end{bmatrix}; B_2^w = \begin{bmatrix} 0 & \gamma_c^1 \\ \vdots & \vdots \\ 0 & \gamma_c^N \end{bmatrix} \tag{A.130}$$

The parameters that appears in equations (A.127) to (A.130) were defined in order to simplify the notation, and they corresponding relation with the process variables are presented in Table A.1.

Table A.1: Definition of parameters for State-Space Model.

a_h^i	b_h^i	c_h^i	d_h^i
$-\alpha_h^i - \beta_h^i \left(\frac{\partial \Delta T_{ef}}{\partial T_h^i}\right)$	$\alpha_h^i - \beta_h^i \left(\frac{\partial \Delta T_{ef}}{\partial T_h^{i-1}}\right)$	$-\beta_h^i \left(\frac{\partial \Delta T_{ef}}{\partial T_c^i}\right)$	$-\beta_h^i \left(\frac{\partial \Delta T_{ef}}{\partial T_c^{i+1}}\right)$
a_c^i	b_c^i	c_c^i	d_c^i
$\beta_c^i \left(\frac{\partial \Delta T_{ef}}{\partial T_h^i}\right)$	$\beta_c^i \left(\frac{\partial \Delta T_{ef}}{\partial T_h^{i-1}}\right)$	$-\alpha_c^i + \beta_c^i \left(\frac{\partial \Delta T_{ef}}{\partial T_c^i}\right)$	$\alpha_c^i + \beta_c^i \left(\frac{\partial \Delta T_{ef}}{\partial T_c^{i+1}}\right)$

Where the following constants are defined:

$$\alpha_h^i = \frac{w_h}{\rho_h V_h^i C p_h}; \;\; \beta_h^i = \frac{UA^i}{\rho_h V_h^i C p_h}; \; \gamma_h^i = \frac{T_h^{i-1} - T_h^i}{\rho_h V_h^i C p_h} \tag{A.131}$$

$$\alpha_c^i = \frac{w_c}{\rho_c V_c^i C p_c}; \;\; \beta_c^i = \frac{UA^i}{\rho_c V_c^i C p_c}; \; \gamma_c^i = \frac{T_c^{i+1} - T_c^i}{\rho_h V_h^i C p_h} \tag{A.132}$$

And the derivative of effective temperature approach:

Table A.2: Partial derivatives of temperature approach.

	$\frac{\partial \Delta T_{ef}}{\partial T_h^i}$	$\frac{\partial \Delta T_{ef}}{\partial T_h^{i-1}}$	$\frac{\partial \Delta T_{ef}}{\partial T_c^i}$	$\frac{\partial \Delta T_{ef}}{\partial T_c^{i+1}}$
$Pure\ Mixing\ Tank$	1	0	-1	0
$AMTD$	$1/2$	$1/2$	$-1/2$	$-1/2$
$LMTD$	$\frac{\partial LMTD}{\partial T_h^i}$	$\frac{\partial LMTD}{\partial T_h^{i-1}}$	$\frac{\partial LMTD}{\partial T_c^i}$	$\frac{\partial LMTD}{\partial T_c^{i+1}}$

A.5 HEN State Space Model

The state space model described by the equations (A.122) and (A.123) and its related definitions is applicable to each heat exchanger in a HEN. Selecting a sequence of N_e heat exchangers, with the model for the ith heat exchanger, named E_i, in a network can be obtained directly by lumping all unit models in the sequence of exchanger numbers, in the same manner it was made to the static case.

$$\frac{d}{dt}\begin{bmatrix}\delta T_{h_{E_1}}^{i,out}\\ \delta T_{c_{E_1}}^{i,out}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{i,out}\\ \delta T_{c_{E_{Ne}}}^{i,out}\end{bmatrix} = [A^*]\begin{bmatrix}\delta T_{h_{E_1}}^{i,out}\\ \delta T_{c_{E_1}}^{i,out}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{i,out}\\ \delta T_{c_{E_{Ne}}}^{i,out}\end{bmatrix} + [B^{t*}]\begin{bmatrix}\delta T_{h_{E_1}}^{in}\\ \delta T_{c_{E_1}}^{in}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{in}\\ \delta T_{c_{E_{Ne}}}^{in}\end{bmatrix} + [B^{w*}]\begin{bmatrix}\delta w_{h_{E_1}}\\ \delta w_{c_{E_1}}\\ \vdots\\ \delta w_{h_{E_{Ne}}}\\ \delta w_{c_{E_{Ne}}}\end{bmatrix} + [B^{u*}]\begin{bmatrix}\delta u_{h_{E_1}}\\ \delta u_{c_{E_1}}\\ \vdots\\ \delta u_{h_{E_{Ne}}}\\ \delta u_{c_{E_{Ne}}}\end{bmatrix} \tag{A.133}$$

$$\begin{bmatrix}\delta T_{h_{E_1}}^{out}\\ \delta T_{c_{E_1}}^{out}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{out}\\ \delta T_{c_{E_{Ne}}}^{out}\end{bmatrix} = C_m^*\begin{bmatrix}\delta T_{h_{E_1}}^{i,out}\\ \delta T_{c_{E_1}}^{i,out}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{i,out}\\ \delta T_{c_{E_{Ne}}}^{i,out}\end{bmatrix} + D_m^{t*}\begin{bmatrix}\delta T_{h_{E_1}}^{in}\\ \delta T_{c_{E_1}}^{in}\\ \vdots\\ \delta T_{h_{E_{Ne}}}^{in}\\ \delta T_{c_{E_{Ne}}}^{in}\end{bmatrix} + D_m^{w*}\begin{bmatrix}\delta w_{h_{E_1}}\\ \delta w_{c_{E_1}}\\ \vdots\\ \delta w_{h_{E_{Ne}}}\\ \delta w_{c_{E_{Ne}}}\end{bmatrix} + D_m^{u*}\begin{bmatrix}\delta u_{h_{E_1}}\\ \delta u_{c_{E_1}}\\ \vdots\\ \delta u_{h_{E_{Ne}}}\\ \delta u_{c_{E_{Ne}}}\end{bmatrix} \tag{A.134}$$

In order to avoid repetitive notation, the matrix M is defined by the equation

$$M = A^* \vee B^{t*} \vee B^{w*} \vee B^{u*} \vee C_m^* \vee D_m^{t*} \vee D_m^{w*} \vee D_m^{u*} \tag{A.135}$$

$$M^* = diag\{M_{E_1}, M_{E_2}, \dots, M_{E_{Ne}}\} \tag{A.136}$$

The system composed by the equations (A.133) and (A.134) can be re-written in the following manner:

$$\frac{d}{dt}\begin{bmatrix}\delta T^{iT}\\ \delta T^{im}\end{bmatrix} = \begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix}\begin{bmatrix}\delta T^{iT}\\ \delta T^{im}\end{bmatrix} + \begin{bmatrix}B_{11}^t & B_{12}^t\\ B_{21}^t & B_{22}^t\end{bmatrix}\begin{bmatrix}\delta T^{S}\\ \delta T^{m}\end{bmatrix} + \begin{bmatrix}B_1^w\\ B_2^w\end{bmatrix}\delta w + \begin{bmatrix}B_1^u\\ B_2^u\end{bmatrix}\delta u \tag{A.137}$$

$$\begin{bmatrix}\delta T^{T}\\ \delta T^{m}\end{bmatrix} = \begin{bmatrix}C_{11} & C_{12}\\ C_{21} & C_{22}\end{bmatrix}\begin{bmatrix}\delta T^{iT}\\ \delta T^{im}\end{bmatrix} + \begin{bmatrix}D_{11}^t & D_{12}^t\\ D_{21}^t & D_{22}^t\end{bmatrix}\begin{bmatrix}\delta T^{S}\\ \delta T^{m}\end{bmatrix} + \begin{bmatrix}D_1^w\\ D_2^w\end{bmatrix}\delta w + \begin{bmatrix}D_1^u\\ D_2^u\end{bmatrix}\delta u \tag{A.138}$$

where

$$\delta T^{iT} = \begin{bmatrix}\delta T_{H1}^{iT} & \dots & \delta T_{HN_h}^{iT} & \delta T_{C1}^{iT} & \dots & \delta T_{CN_c}^{iT}\end{bmatrix}^T \tag{A.139}$$

$$\delta T^{im} = \begin{bmatrix}\delta T_1^{im} & \dots & \delta T_{N_m}^{im}\end{bmatrix}^T \tag{A.140}$$

and all the other vector have been already defined in (A.99) to (A.103). The rewritten model can be related with the original by the following equations:

$$\begin{bmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{bmatrix} = V_1^i A^* \left(V_1^i\right)^T; \quad \begin{bmatrix}B_{11}^t & B_{12}^t\\ B_{21}^t & B_{22}^t\end{bmatrix} = V_1^i B^{t*} V_2 \tag{A.141}$$

$$\begin{bmatrix}B_1^w\\ B_2^w\end{bmatrix} = V_1^i B^{w*} V_3; \quad \begin{bmatrix}B_1^u\\ B_2^u\end{bmatrix} = V_1^i B^{u*} V_4 \tag{A.142}$$

$$\begin{bmatrix}C_{11} & C_{12}\\ C_{21} & C_{22}\end{bmatrix} = V_1 C_m^* \left(V_1^i\right)^T; \quad \begin{bmatrix}D_{11}^t & D_{12}^t\\ D_{21}^t & D_{22}^t\end{bmatrix} = V_1 D_m^{t*} V_2 \tag{A.143}$$

$$\begin{bmatrix} D_1^w \\ D_2^w \end{bmatrix} = V_1 D_m^{w*} V_3; \; \begin{bmatrix} D_1^u \\ D_2^u \end{bmatrix} = V_1 D_m^{u*} V_4 \tag{A.144}$$

The derivation of the matrix V_1^i is made in the next topic. For instance consider the conversion of the state space model in the appropriated one, with inputs and outputs without the intermediate temperatures. First, the equation (A.138) is separated into two new equations

$$\delta T^T = C_{11}\delta T^{iT} + C_{12}\delta T^{im} + D_{11}^t \delta T^S + D_{21}^t \delta T^m + D_1^w \delta w + D_1^u \delta u \tag{A.145}$$

$$\delta T^m = C_{21}\delta T^{iT} + C_{22}\delta T^{im} + D_{21}^t \delta T^S + D_{22}^t \delta T^m + D_2^w \delta w + D_2^u \delta u \tag{A.146}$$

Maintaining the state vector to describe the system, it is obtained an expression for the intermediate temperature vector

$$(I - D_{22}^t)\delta T^m = C_{21}\delta T^{iT} + C_{22}\delta T^{im} + D_{21}^t \delta T^S + D_2^w \delta w + D_2^u \delta u \tag{A.147}$$

$$\delta T^m = (I - D_{22}^t)^{-1} \left\{ [C_{21} \quad C_{22}] \begin{bmatrix} \delta T^{iT} \\ \delta T^{im} \end{bmatrix} + D_{21}^t \delta T^S + D_2^w \delta w + D_2^u \delta u \right\} \tag{A.148}$$

Substituting the equation (A.148) in (A.37) and (A.145), it is possible to obtain the expressions (A.149) and (A.150) respectively, which represent the state space model of the HEN

$$\frac{d}{dt}\begin{bmatrix} \delta T^{iT} \\ \delta T^{im} \end{bmatrix} = A_o \begin{bmatrix} \delta T^{iT} \\ \delta T^{im} \end{bmatrix} + B_o^t [\delta T^S] + B_o^w \delta w + B_o^u \delta u \tag{A.149}$$

$$\delta T^T = C_o \begin{bmatrix} \delta T^{iT} \\ \delta T^{im} \end{bmatrix} + D_o^t \delta T^S + D_o^w \delta w + D_o^u \delta u \tag{A.150}$$

where

$$C_o = [C_{21} \quad C_{22}] + D_{12}^t (I - D_{22}^t)^{-1} [C_{21} \quad C_{22}] \tag{A.151}$$

$$D_o^t = D_{11}^t + D_{12}^t (I - D_{22}^t)^{-1} D_{21}^t \tag{A.152}$$

$$D_o^w = D_1^w + D_{12}^t (I - D_{22}^t)^{-1} D_2^w \tag{A.153}$$

$$D_o^u = D_1^u + D_{12}^t (I - D_{22}^t)^{-1} D_2^u \tag{A.154}$$

and

$$A_o = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} + \begin{bmatrix} B_{12}^t \\ B_{22}^t \end{bmatrix} (I - D_{22}^t)^{-1} [C_{21} \quad C_{22}] \tag{A.155}$$

$$B_o^t = \begin{bmatrix} B_{11}^t \\ B_{21}^t \end{bmatrix} + \begin{bmatrix} B_{12}^t \\ B_{22}^t \end{bmatrix} (I - D_{22}^t)^{-1} D_{21}^t \tag{A.156}$$

$$B_o^w = \begin{bmatrix} B_1^w \\ B_2^w \end{bmatrix} + \begin{bmatrix} B_{12}^t \\ B_{22}^t \end{bmatrix} (I - D_{22}^t)^{-1} D_2^w \tag{A.157}$$

$$B_o^u = \begin{bmatrix} B_1^u \\ B_2^u \end{bmatrix} + \begin{bmatrix} B_{12}^t \\ B_{22}^t \end{bmatrix} (I - D_{22}^t)^{-1} D_2^u \tag{A.158}$$

From the state space model the following transfer function matrices can be derived:

$$G_u(s) = C_o(Is - A_o)^{-1}B_o^u + D_o^u \tag{A.159}$$

$$G_d^t(s) = C_o(Is - A_o)^{-1}B_o^t + D_o^t \tag{A.160}$$

$$G_d^w(s) = C_o(Is - A_o)^{-1}B_o^w + D_o^w \tag{A.161}$$

And the general transfer function model:

$$\delta T^T(s) = G_u(s)\delta T^S(s) + G_d^t(s)\delta w(s) + G_d^w(s)\delta u(s) \tag{A.162}$$

To complete the description of the state space and transfer function model, it is necessary define the matrix V_1^i.

$\underline{Derivation\ of}$ V_1^i. Each element of matrix V_1^i has a value 0 or 1 relating the disordered vector δT_E^{out} with the ordered vector $[\delta T^{iT} \quad \delta T^{im}]^T$. Fist, the matrix V_1^i must have all elements set to 0. The first row of V_1^i (i) that corresponds to the $\delta T_{h1}^{iT}(1)$ relation, considering that this target is located in the k position in the disordered vector, set $V_1^i(i,k)$=1. For the number of cells used to described the dynamic behavior of the heat exchanger N set $V_1^i(i+j,k+j)$=1 with $j = \{1, \dots, N-1\}$. In case of the target temperature is a mixed stream; the vector δT^{iT} is substituted by the composed vector δT_{mixed}^{iT} and the mixing effect is computed by the V_1 matrix, where $\delta T_{mixed}^{iT} = [\delta T_{branch1}^{iT} \quad \dots \quad \delta T_{branchNb}^{iT}]$.

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Appendix B

Operational Flexibility and Controllability of Heat Exchanger Networks

***Abstract**: Operability considerations, such as flexibility and controllability are very important in a HEN design, but they are usually neglected during the design phase for a given steady state operating point. The HEN structure introduces interactions and dramatically change the plant dynamics, and it may make the process more difficult to control and operate. For a given HEN it is necessary to evaluate its ability to achieve feasible operation over a range of conditions while satisfying performance specifications, regarded as flexibility. It is also important to have a strategy for operating and control those results in reasonable dynamic performance of the plant. For a fixed design it is necessary to perform a flexibility and controllability analysis, intrinsically related to the optimal operation. This Chapter addresses the flexibility and controllability analysis of designed HENs. It is separated into two parts. In the former, a flexibility analysis is performed for a case study with five different structures. In the latter, the qualified HENs (flexible) go through a controllability analysis where the control structure selection is defined and the nominal bypasses are designed.*

Nomenclature

Abbreviations	
FI	*flexibility index*
$FCHR$	*feasible convex hull ratio*
HEN	*heat exchanger network*
$HENS$	*heat exchanger network synthesis*
$HRAT$	*heat recovery approach temperature*
$LMTD$	*log mean temperature difference*
LP	*linear programming*
MER	*maximum energy recovery*
$MILP$	*mixed integer linear programming*
$MINLP$	*mixed integer non linear programming*
NLP	*nonlinear programming*
RI	*resilience index*
SF	*stochastic flexibility*
TAC	*total annual cost*

Sets	
CP	*set of cold process stream j*
HU	*set of hot process stream i*
V	*set of periods n*

Variables	*Units*	
G_u		*gain matrix from bypass fraction to target temperatures*
G_t^d	[°C]	*gain matrix from supply temperature to target temperatures*
G_w^d	[kW/K]	*gain matrix from flowrate capacity to target temperatures*
$G_t^{d^h}$	[°C]	*gain matrix from hot supply temperature to target temperatures*
$G_t^{d^c}$	[°C]	*gain matrix from cold supply temperature to target temperatures*
$G_w^{d^h}$	[°C]	*gain matrix from hot flowrate capacity to target temperatures*
$G_w^{d^c}$	[°C]	*gain matrix from cold flowrate capacity to target temperatures*
a		*constant definition for heat exchanger model*
δ		*scaled factor for uncertain parameters description*
δ^*		*flexibility index*
T_h^{in}	[°C]	*inlet temperature of hot stream i*
T_c^{in}	[°C]	*inlet temperature of cold stream j*
T_h^{out}	[°C]	*outlet temperature of hot stream i*
T_c^{out}	[°C]	*outlet temperature of cold stream j*
$T_{i,n}^{out}$	[°C]	*outlet temperature of hot stream i at period n*
$T_{j,n}^{out}$	[°C]	*outlet temperature of cold stream j at period n*
$T_{i-1,n}^{out}$	[°C]	*outlet temperature of hot stream i at period n before utility unit*

$T_{j-1,n}^{out}$	[°C]	*outlet temperature of cold stream j at period n before utility unit*
$\delta q_{Hi,n}^{CU}$	[kW]	*cold utility heat load for hot stream i*
$\delta q_{Cj,n}^{HU}$	[kW]	*hot utility heat load for cold stream j*
δT^{t}	[°C]	*target temperature deviation*
δT^{s}	[°C]	*supply temperature deviation*
δw	[°C]	*flowrate capacity deviation*
δu	[°C]	*bypass fraction deviation*
w_h	[kW/K]	*flowrate capacity of hot stream*
w_c	[kW/K]	*flowrate capacity of cold stream*
u_h		*bypass fraction for hot side*
u_c		*bypass fraction for cold side*
u_{lim}		*upper bound for bypass fraction*
u_{nom}		*nominal bypass fraction*
u_{opt}		*optimal bypass fraction*
u_k^{lim}		*upper bound for bypass fraction k*
R_h		*flowrate ratio*

Parameters	*Units*	
A	[m^2]	*heat exchanger area*
A_0	[m^2]	*original heat exchanger area*
δA	[m^2]	*heat exchanger area variation*
Q	[kW]	*heat load of heat exchanger*
δT^{t}	[m^2]	*Target temperature deviation*
$\delta T^{s(+)}$	[°C]	*positive expected deviation of supply temperature*
$\delta T^{s(-)}$	[°C]	*negative expected deviation of supply temperature*
$\delta T_{max}^{t(+)}$	[°C]	*positive accepted deviation of target temperature*
$\delta T_{max}^{t(-)}$	[°C]	*negative accepted deviation of target temperature*
$\delta w^{(+)}$	[kW/K]	*positive expected deviation of flowrate capacity*
$\delta w^{(-)}$	[kW/K]	*negative expected deviation of flowrate capacity*
$\delta T^{s(+)^{c}}$	[°C]	*positive expected deviation of cold supply temperature*
$\delta T^{s(+)^{h}}$	[°C]	*positive expected deviation of hot supply temperature*
$\delta T^{s(-)^{c}}$	[°C]	*negative expected deviation of cold supply temperature*
$\delta T^{s(-)^{h}}$	[°C]	*negative expected deviation of hot supply temperature*
$\delta w^{(+)^{c}}$	[kW/K]	*positive expected deviation of cold flowrate capacity*
$\delta w^{(+)^{h}}$	[kW/K]	*positive expected deviation of hot flowrate capacity*
$\delta w^{(-)^{c}}$	[kW/K]	*negative expected deviation of cold flowrate capacity*
$\delta w^{(-)^{h}}$	[kW/K]	*negative expected deviation of hot flowrate capacity*

β	-	*exponent for the area cost for heat exchanger cost estimation*
c_{cu}	[\$/kW.yr]	*utility cost coefficient for cooling utility*
c_{hu}	[\$/kW.yr]	*utility cost coefficient for heating utility*
a	[\$/kW.yr]	*Fixed cost for heat exchanger cost estimation*
b	[\$/kW.yr]	*variable cost for heat exchanger cost estimation*
w	[kW/K]	*flow capacity of hot/cold stream*
T_{in}	[°C]	*inlet temperature of process stream*
h	[kW/m²K]	*heat transfer coefficient for process stream*
ΔT_{min}	[°C]	*minimum temperature approach*
T_{in}	[°C]	*inlet temperature of process stream*
T_{out}	[°C]	*outlet temperature of process stream*
$T_{i,n}^{in}$	[°C]	*inlet temperature of hot stream i at period n*
$T_{j,n}^{in}$	[°C]	*inlet temperature of cold stream j at period n*
$T_{i,0}^{in}$	[°C]	*inlet temperature of hot stream i at nominal condition*
$T_{j,0}^{in}$	[°C]	*inlet temperature of cold stream j at nominal condition*
T_i^{sp}	[°C]	*reference or setpoint value for hot stream i*
T_j^{sp}	[°C]	*reference or setpoint value for cold stream j*
n		*rank of matrix energy balance*
n_b		*number of bypasses to be placed*
$n_{dof,u}$		*number of degrees of freedom for utility optimization*
n_{hx}		*number of heat exchangers of the HEN*
n_u		*number of utility units of the HEN*
n_s		*number of process streams of the HEN*
N		*number of uncertain parameters*
NH, NC		*number of hot,cold streams*
V		*number of vertices of the polyhedral region of uceratinty*
$r_{i,n}$		*disturbance direction identifier for hot stream i at period n*
$r_{j,n}$		*disturbance direction identifier for cold stream j at period n*
$w_{h,i}$		*flowrate capacity of hot stream i*
$w_{c,j}$		*flowrate capacity of cold stream j*
T_j^{out}		*outlet temperature of cold stream j*
δ		*scaled factor for uncertain parameters description*
δ_T		*Flexibility target for uncertain parameter*
θ		*uncertain parameter*
θ^N		*uncertain parameter at nominal condition*
$\Delta\theta^+$		*positive expected deviation of uncertain parameter*
$\Delta\theta^-$		*negative expected deviation of uncertain parameter*
$\omega_{i,j}$	-	*weights to the match i-j*

Operational Flexibility of Heat Exchanger Networks

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Abstract Process integration is motivated from economic benefits, but it also impacts on the plant behavior introducing interactions and in many cases making the process more difficult to control and operate. A prerequisite for optimal operation is that the HEN is sufficiently flexible, i.e. it must have the ability to operate over a range of conditions while satisfying performance specifications. In this work it is defined the Operational Flexibility related not only to the size of the feasible region but also to the costs involved to put the HEN into operation. In order to provide an appropriated metric, the operational flexibility index is defined. Five different networks structures designed for the nominal conditions of a case study are used to illustrate the proposed ideas. It was noticed that a great feasible region does not point out the more economic operation, and the costs must be considered together with the flexibility analysis. These characteristics are taken into account by the novel proposed operational flexibility index, which can also consider during the analysis the increasing in the utility duties, extra utility exchangers and bypass installation. These results clearly point out for the need of a simultaneous framework for flexible design and profitability.

Keywords: Heat Exchanger Networks, Optimal Operation, Operational Flexibility.

1. INTRODUCTION

Operability issues are very important for heat integrated process, since the economic performance of a process is greatly affected by process variations and the ability of the system to satisfy its operational specifications under external disturbances or inherent modelling uncertainty.

Methods based on pinch analysis and mathematical programming for fixed operating conditions hve been largely developed. An extensive review of these methods can be found in Furman and Sahinidis (2002). Compared to design of HENs for nominal operating conditions, less effort has been dedicated to the operability and controllability aspects of such networks.

Since the concept of resilient HENs firstly developed by Marselle et al. (1982) and the introduction of the flexibility index by Swaney and Grossmann (1985) several design methods based on the multiperiod approach were proposed. Floudas and Grossmann (1986) introduced a multiperiod case based on the synthesis with decomposition. Papalexandri and Pistikopoulos (1994) and Konukman et al. (2002) extended the simultaneous synthesis to the multiperiod case in an MINLP problem.

All these works relates the flexibility with the size of the feasible region and they do not take into account explicitly all the trade-offs involved in a HEN design. In this work a new metric for comparing different HEN structures is proposed based on the concept of operational flexibility. A case study with 5 different synthesized HENs is used to illustrate the proposed metric.

2. OPERATION OF HENs

A HEN is considered optimal operated if the targets temperatures are satisfied at steady state (main objective); the utility cost is minimized (secondary goal); and the dynamic behaviour is satisfactory (Glemmestad, 1997).

During HEN operation, degrees of freedom or manipulated inputs are needed for control and optimization. The different possibilities are shown in Figure 1: 1-Utility Flowrates; 2-Bypass fraction; 3-Split fraction; 4-Process Streams flowrates; 5-Exchanger area (e.g. flooded condenser); 6-Recycle (e.g. if exchanger fouling is reduced by increased flowrates).

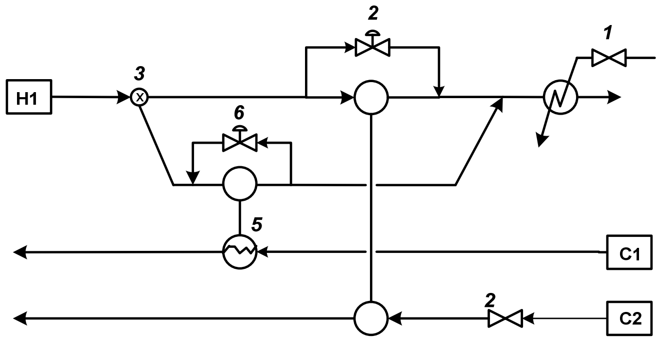

Fig. 1. Possible manipulated inputs in HENs.

In this work, we will consider the outlet target temperatures as controlled variables and utility loads, bypasses or splits, when they are present, as manipulated variables. The idea is to maintain the targets temperatures using the minimal increase of the external utilities. The best HEN is the one where the effect of a given set of disturbances can be accommodated internally without requiring too much external "help" from the utilities heat exchangers. These ideas are illustrated through the case study of the next section.

3. CASE STUDY

To analyze the flexibility problem we have synthesized 5 different HENs for the plant illustrated in Figure 2.

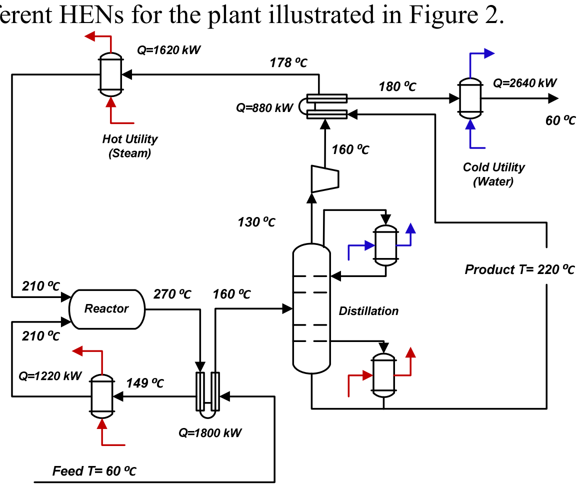

Fig. 2. Simple process with reaction, separation and heat exchangers.

Table 1. Nominal operating condition for the Case Study.

Stream	T_{in} (ºC)	T_{out} (ºC)	*F* (kWºC^{-1})	*h* (kW m^2 ºC^{-1})
H1	270	160	18	1
H2	220	60	22	1
C1	50	210	20	1
C2	160	210	50	1
CU	15	20		1
HU	250	250		1

Cost of Heat Exchangers (\$y^{-1}) = 4000+500[Area (m^2)]$^{0.83}$
Cost of Cooling Utility = 20 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 200 (\$kW^{-1}y^{-1})

Table 1 summarizes the corresponding data of the nominal operating conditions. This data and a ΔT_{min} of 10 ºC were used to design the 5 different HENs depicted in Fig. 3. The five HENs have been designed by the following approaches:

S01-Pinch Technology (Linnhoff & Hindmarsh, 1983);

S02-NLP Superstructure proposed by Floudas, Ciric, and Grossmann (1986) using Pinch Technology as initial guesses;

S03-NLP Superstructure in the Sequential procedure (Floudas, Ciric, and Grossmann, 1986);

S04-Hyperstrucutre proposed by Ciric and Floudas (1991); and

S05- the stage-wise Synheat model proposed by Yee and Grossmann (1990) with the assumption isothermal mixing.

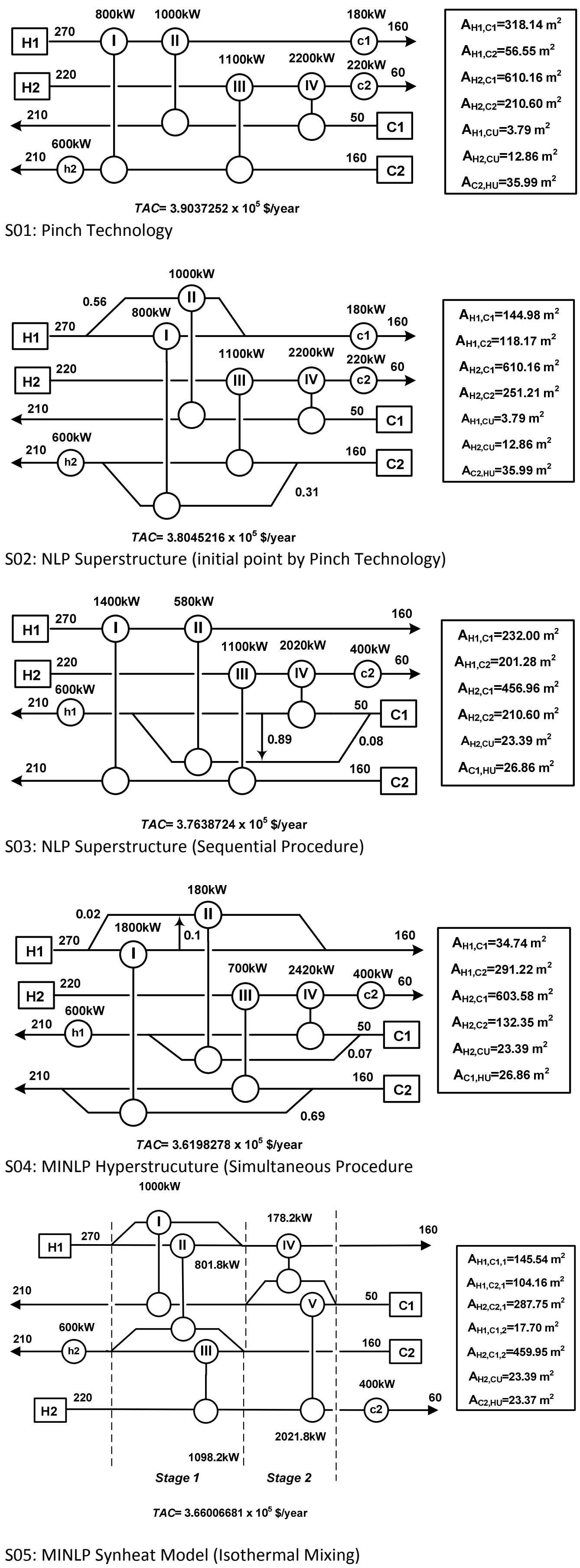

Fig. 3. Synthesized HENs for the Case Study using different approaches.

4. OPERATIONAL FLEXIBILITY

The flexibility is defined by Swaney and Grossmann (1985) as the size of the region of feasible operation in the space of possible deviations of the parameters from their nominal values. In order to analyze the flexibility, a disturbance scenario is explored on the basis of the vertices of the polyhedral region of uncertainty (Konukman et al., 2002) trough a scalar δ (flexibility target). For a fixed HEN topology and design the 'flexibility index' is defined by Swaney and Grossmann (1985) as the maximum scalar δ* (Figure 4).

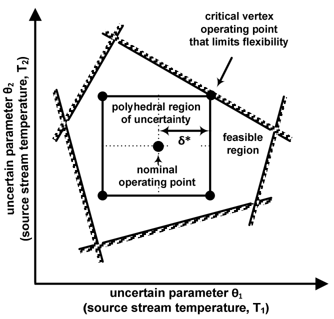

Fig. 4. Geometric representation of vertex-based flexibility target.

As the feasible region is convex when it is considered the inlet temperatures as uncertain parameters, the critical point that limits the operation lies at a vertex of the polyhedral region of uncertainty. For non-convex region the vertex-based formulation should be replaced by a more general active-constraint-strategy-based on MINLP formulation (Floudas, 1995).

Considering the four inlet temperatures as disturbances, a total of 16 vertices are enumerated. Each vertex represents an operating condition and it is formed by a deviation of ±δ from the nominal values In order to calculate the expected variations in the operating conditions that potentially could happen for a given flexibility target, each HEN configuration was implemented in Excel® using the heat exchanger model described by the set of equations (1), (2), and (3) and notation shown in Fig. 5.

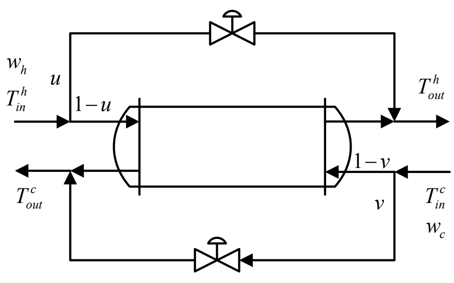

Fig. 5. General structure of a heat exchanger with bypasses.

$$T_{out}^{h} = (1-u)\left[\frac{(R_h-1)}{R_h-a}T_{in}^{h} + \frac{(1-a)}{R_h-a}T_{in}^{c}\right] + uT_{in}^{h} \tag{1}$$

$$T_{out}^{c} = (1-v)\left[\frac{R_h(1-a)}{R_h-a}T_{in}^{h} + \frac{a(R_h-1)}{R_h-a}T_{in}^{c}\right] + vT_{in}^{c} \tag{2}$$

Where

$$R_h = \frac{w_h(1-u)}{w_c(1-v)}; NTU_h = \frac{UA}{w_h(1-u)}; a = e^{NTU_h(1-R_h)} \tag{3}$$

The individual heat exchanger model was connected according to the topology for each HEN structure and the outlet temperatures deviations from their target values are calculated together with the additional utility requirement. A free simulation for fixed bypass and split fractions was carried out for each operating condition. Positive values encountered of heat duties at the stream where no utility exchanger exist mean that an extra utility exchanger must be included. Moreover, the negative values indicate an infeasible operation without any structural modifications, even for adding a new utility exchanger.

4.1 Optimal Operation of HENs

To overcome an infeasible operation it is possible to use the degrees of freedom, such as split fractions and bypasses placement in order to increase the feasible region and ensure that the optimal operation can be achieved by minimizing the utility consumption. The optimal steady-state operation or network optimization problem (Marselle et al., 1982):

Optimal Steady State Operation: *(For each operating point n)*

*Minimum Utility Consumption (**secondary objective**)*

$$\min_{u,v} \sum_{i=1}^{NH} Q_{i,n}^{CU} + \sum_{j=1}^{NC} Q_{j,n}^{HU}$$

subject to.

*Hot and Cold target temperatures (**primary goal**)*

$$T_{i,n}^{out} - T_i^{sp} = 0; T_{j,n}^{out} - T_j^{sp} = 0$$

Positives or zero heat loads coolers and heaters

$$T_i^{sp} - T_{i-1,n}^{out} \le 0; T_{j,n}^{out} - T_j^{sp} = 0$$

Hot and Cold Utility loads

$$Q_{i,n}^{HU} = w_i^H\left(T_{i-1,n}^{out} - T_{i,n}^{out}\right)$$

$$Q_{j,n}^{CU} = w_j^C\left(T_{j,n}^{out} - T_{j-1,n}^{out}\right)$$

Heat Exchanger Static Model

(3), (4), and (5)

*Topology Constraints**

Bypass bounds

$$0 \le u, v \le 1$$

** The topology constraints define the configuration, and are expressed as appropriated model variables connections.*

The optimal optimization problem for each configuration was implemented using the software GAMS and solved using the solver CONOPT considering δ_T is equal to 10°C (flexibility target). The new requirements for the each HEN structure are exhibited in Table 2.

According to the initial analysis, the maximum or critical utility exchanger operation is not a good metric since it was not able to distinguish the configurations S01 and S02. Furthermore, comparing the configurations S03 and S04, even though the critical loads are greater for the first one the total heat load (summation for each operation point) and the averages are not.

Table 2. Utility loads (kW) for a feasible operation for each case study using extra utility units.

Struc.	Utility	Maximum	Average	Total
S01	cold	1000	446	7584
	hot	1300	646	10984
S02	cold	1000	445	7563
	hot	1300	645	10963
S03	cold	1300	570	9886
	hot	1480	769	13073
S04	cold	1287	586	9966
	hot	1466	782	13306
S05	cold	1000	497	8455
	hot	1480	696	11840

According to the results the configurations S03 and S04 are the worst from a flexibility point of view, since they require more utility to a feasible operation. On the other hand, S04 is the HEN with lowest TAC (3.619 x10^5 \$/year) as shown in Fig. 3, but considering the flexibility this is not the best option and clearly points out that flexibility issues must be considered in an early stage of the process design, since the nominal optimum .

4.2 Optimal Operation with no extra utility units

The solution provided in the previous analysis is trivial and may guarantee the operation for a large range. Furthermore, it is an expensive solution. Providing a more reasonable analysis, a second optimal operation problem was considered. The new problem definition differs from the previous one by the addition of constraints that ensure no extra utility exchangers. The general results are presented in Table 3.

Table 3. Utility loads (kW) for a feasible operation for each case study using no extra utility units.

Struc.	Utility	Maximum	Average	Total
S01	cold	1000	494	8425
	hot	1714	694	11825
S02	cold	1003	502	8534
	hot	1540	702	11934
S03*(8)	cold	1058	521	8851
	hot	1480	721	12251
S04*(14)	cold	902	499	8410
	hot	1480	699	11810
S05*(7)	cold	1000	530	9011
	hot	1587	730	12411

* (*ni*) indicate *ni* infeasible operating points.

Due to extra constraints, greater utility consumption in general was need. Moreover, how it was expected not always a feasible solution could be found. The main difficult faced by the configurations S03, S04 and S05 was the presence of only two utility exchangers, i.e. these configurations are more penalized with the additional constraints. The bad performance of the configuration S05 may be also explained possibly by the "inflexible" isothermal mixing constrain applied to the design.

A new analysis was made considering the possibility of variation for the extra degrees of freedom, when they take place. Whereas the configuration S01 has no one split fraction, the best possible results has already presented in Table 3. Conversely, all other configurations have split fractions. For the configurations S03 and S04 was also considered as an extra degree of freedom the recycle stream, from the outlet of a heat exchanger to another. The results are presented in Table 4.

Table 4. Utility loads (kW) for a feasible operation for each case study using no extra utility units but using extra degrees of freedom (split and recycle fractions).

Struc.	Utility	Maximum	Average	Total
S01	cold	1000	494	8425
	hot	1714	694	11825
S02	cold	900	435	7396
	hot	1430	635	10796
S03*(7)	cold	990	458	7780
	hot	1383	658	11180
S04*(8)	cold	780	417	7088
	hot	1368	641	10904
S05	cold	900	456	7745
	hot	1431	656	11145

* (*ni*) indicate *ni* infeasible operating points.

Like it was expected the extra degrees may be used to achieve the targets and decreases the utility consumption increasing the feasible region, which is proven by the increase of the number of feasible operating points. For the configuration S05, allowing the manipulation of the split fractions automatically removes the isothermal mixing assumption and hence increases considerably the flexibility.

Comparing the results, the configurations S03 and S04 must be discarded because they do not provide a suitable operation. The results are a sign of designs with splits are good from the flexibility viewpoint because these extra degrees of freedom can be used to decrease the investment cost during the design phase and be used to decrease the utility consumption during operation. In addition, the installed areas are utilized completely for all operating points, which not occurs using bypasses. In the overall design the dynamic behaviour must be analysed carefully once split fractions can give competitive effects.

4.3 Flexibility Range

All the previous analysis considered the flexibility target (δ_T) of 10ºC, in order to analyze the flexibility range, the total utility consumption (δQ) levels corresponding to the critical operating conditions versus the flexibility targets (δ_T) for structures S01, S02 and S05 and the virtual structure (Maximum Energy Recovery) MER were calculated and they are shown in Figure 6.

The illustration reveals plateaus of total utility requirements levels for a given value of δ, under the correspondent δQ level the configuration is operable, i.e. it will not violate the temperatures specifications as long as the deviations in the source streams temperatures along the vertex directions have magnitudes within $0< \delta_T < \delta$.

The analysis reveals the trade-off between the flexibility target and the total utility load need to maintain a feasible operation pointing out that a more flexible is more expensive. For practical purposes, increasing the flexibility target trough penalization of total utility consumption is possible until a limit (δ*), which is reached when at least one bypass saturation occurs.

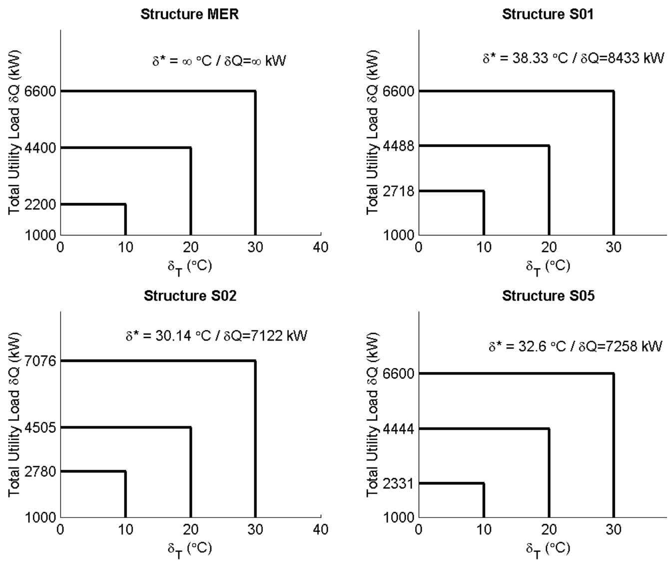

Fig. 6. Total utility consumptions at the critical operating conditions versus the flexibility ranges for structures MER, S01, S02 and S05.

In Table 4, the structure S02 (δ*=38.33^{o}C) depicted the lowest total utility load in general (considering all operating points) and the lowest average utility load. Therein, the critical loads define the feasibility operational range and it must be checked, but a selection of a structure using purely the analysis provided by the Figure 6 will not be appropriated because it would assume that most of the time the process would operate in the critical conditions what is not correct.

5. OPERATIONAL FLEXIBILITY INDEX

An appropriated metric to compare different HENs is based on the operational flexibility that is reached if the operation is possible and the maximum energy recovery is obtained for the entire feasible region with a minimum investment cost.

The structure of the HEN has a direct influence on the flexibility. Disintegrated structures are highly flexible, but that trivial solution is not interesting under an economic point of view. The other highly flexible possibility is a totally integrated structure, with the maximum number of units and maximum areas with bypasses across all units, but very expensive from an investment point of view.

Here we introduce the operational flexibility index to take into account in addition to the feasible range related with a flexibility target the most important costs involved during a "flexible operation". The Operational Flexibility Index for a specific flexibility target (OF_δ) is defined in equation (4), where the two terms correspond to operating cost (φ_{oc}) and the investment cost (φ_{ic}) penalties for an operational flexibility, and these terms are defined in equations (5) and (6). The operational flexibility index varies form 0 to 100%. Its upper bound indicates feasible operation without much economic penalty. On the other hand, when bypasses, new units, increased areas, and increased utility consumption are considered the indice will be penalized.

$$OF_\delta(\%) = 100\left(1-\varphi_{oc}-\varphi_{ic}\right) \tag{4}$$

$$\varphi_{OC} = w_1 \frac{1}{2(V+1)} \sum_{n=1}^{V} \frac{\sum_{k=1}^{NH+NC} \delta q_{k,n}^{U} - \sum_{k=1}^{NH+NC} \delta q_{k,n}^{U,\min}}{\sum_{k=1}^{NH+NC} \delta q_{k,n}^{U,\max} - \sum_{k=1}^{NH+NC} \delta q_{k,n}^{U,\min}} \tag{5}$$

$$\varphi_{IC} = w_2 \frac{N_{bp}}{N_{hx,retrofit}} + w_3\left(1-\frac{N_{hx}}{N_{hx,retrofit}}\right) + w_4\left(N_{hx} - \sum_{m=1}^{N_{hx}} \frac{A_{m,installed}}{A_{m,retrofit}}\right) \tag{6}$$

The parameters w_i (7) correspond to the normalized weight for each contribution to the penalty. A suggested set may be calculated by the constants k_i (8) that depends on economic data from the process, i.e. the utility costs and the exchanger costs, considering the bypass cost. For the case study these parameters are provided in Table 1.

$$w_i = \frac{k_i}{\sum_{i=1}^{4} k_i} \tag{7}$$

$$k_1 = \frac{cu.}{2(V+1)}\left(\sum_{k=1}^{NH+NC} \delta q_{k,n}^{U,\max} - \sum_{k=1}^{NH+NC} \delta q_{k,n}^{U,\min}\right)$$
$$k_2 = 0.2aN_{hx,ret};\ k_3 = aN_{hx,ret};\ k_4 = b\sum_{m=1}^{N_{hx}} A_{m,ret}^{\beta} \tag{8}$$

The parameters N_{bp}, N_{hx} and A_m correspond to the number of bypasses placed, the number of heat exchangers and the area of the heat exchanger *m*, respectively. Moreover, the subscript 'retrofit' indicates the variable in the flexible operation, i.e. the retrofitted design.

To evaluate the potential of each structure, the operational flexibility index was calculated. The calculation requires the bounds for the utility loads. It was used the LP transshipment model (Papoulias and Grossmann, 1983) for each operating point to estimate the minimum utility consumption for the design case (ΔT_{min}=10^{o}C) and the minimum case (ΔT_{min}=0^{o}C). Furthermore, it was calculated the utility loads for the no heat integration case; all the targets are exhibited in Table 5.

Table 5. Utility loads (kW) for a feasible operation for each case study using no extra utility units.

Case	*Utility*	*Max.*	*Average*	*Total*
MER	*cold*	900	412	7000
ΔT_{min}=10^{o}C	*hot*	1300	612	10400
MER	*cold*	900	219	3720
ΔT_{min}=0^{o}C	*hot*	1080	360	6120
No Heat	*cold*	5900	5500	93500
Integration	*hot*	6400	5700	96900

The main results are expressed in Table 6. The term corresponding to the energy cost is dominant due to its greater economic impact in the total cost; the investment cost is worthless for most cases. The structure S02 showed the best performance for the required flexibility target. The interpretation inside the context of a feasible operation is that a greater index indicates that operation occurs inside a more economic way, using a lower average utility consumption with the lower investment cost. Otherwise different conditions will penalize the operational flexibility.

Table 6. Operational Flexibility Index for the structures S01, S02 and S05.

	S01	***S02***	***S05***
φ_{oc}	0.0605691	0.0498255	0.0536638
φ_{ic}	0.00203939	0.00271918	0.00000000
$OF_{\delta=10}$	93.73916%	94.74553%	94.63362%

5.1 Flexibility x Installed Area

All the previous analysis was carried out using the areas as fixed parameters, and these areas were designed at nominal conditions. If it was considered the whole feasible region, trough a multi-period design these areas would have better usage in order to reduce the utility consumption in the entire region. A new optimization problem was performed for the structure S01, considering varying areas. In order to avoid extreme solutions, a practical consideration for the areas bounded between 1 and 1000 m^2 were imposed and new optimizations were performed. The areas for each operating point are presented in Table 7. In order to satisfy all operating points, the maximum areas obtained in Table 7 where fixed and the optimal operation problem was solved with the increased areas.

Table 7. Nominal and maximum areas (m^2) for the HEN structure S01.

	$A_{H1,C1}$	$A_{H1,C2}$	$A_{H2,C1}$	$A_{H2,C2}$
Nominal	318.12	56.55	609.97	209.79
Maximum	1000.00	97.46	1000.00	1000.00

Comparing the values obtained with the results presented in Table 4 for the structure S01, the total utility loads decreased from 8425.3kW to 4370.9 kW (cold utility) and 11825.3 kW to 7770.9 kW (hot utility); and the average consumption decreased from 494kW to 257kW(cold utility) and 694kW to 457kW (hot utility). The flexibility index (δ*) provided in the Figure 6 increased from 38.33^{0}C to 49.8^{0}C, i.e. the feasible region increased. Furthermore, the operational flexibility index (OF_δ) exhibited in Table 6 increased from 93.73916% to 98.197858% considering only the energy cost and considering the capital cost for the oversize of the areas the index is 97.02954%.

6. CONCLUSIONS

The flexibility analysis of different structures previously designed was accomplished through optimal operation problem taking into account the trade-offs between energy cost, capital cost and the flexibility in order to ensure an economic operation. The formulation presumed that the feasible region in the space of uncertain input parameters was convex, and thus the optimal solution was explored based on the vertices of the polyhedral uncertainty region in the space of source-stream temperatures. It was defined the operational flexibility index as a measure of operational flexibility that was assumed to be different of structural flexibility. The first one considers the impacts on the total annual cost, since infinity areas, high levels of utility loads and disintegrated structures are according with this work highly structural flexible but present a poor (expensive) operation and hence a low operational flexibility.

The HEN structure provides an upper bound for the flexibility that should be expected during operation. The increasing of flexibility target reveals the flexibility dependent on structural modifications and total utility consumption until the unfeasible operation may be achieved. It was showed that more important that the size of the feasible region it is the cost involved in a feasible operation around the desired flexibility target. It has shown the real need of taking into account the flexibility in a simultaneous framework, once the utility loads, heat exchangers (units and areas), and the arrange (configuration of flows, temperatures) are determined in only one step, and all these variables strongly affect the flexibility.

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Operational Controllability of Heat Exchanger Networks

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Abstract: Process integration is motivated from economic benefits, but it also impacts on the plant behavior introducing interactions and in many cases making the process more difficult to control and operate. During the operation utility flow rates and bypasses are widely used for effective control of process stream target temperatures, but the number of utility units is usually less than the number of process streams in the network and some bypasses should be selected. This paper addresses the optimal bypass design for heat exchanger networks. It consists in a model-based iterative procedure considering controllability metrics and worst-case disturbance rejection with minimum economic penalty. This is essentially a piecewise linearization approach producing excellent results. The methodology proposed is demonstrated using a case study with 3 different structures, making possible a comparison among different options on a quantitative basis, taking into account the optimal operation attainable with minimum total annual cost. These results clearly point out for the need of a simultaneous framework for design with controllability and profitability. The main goal of this work is to contribute within the field of optimal operation and control of HENs and the definition of the operational controllability concept.

Keywords: Heat Exchanger Networks, Optimal Operation, Operational Controllability.

1 INTRODUCTION

Operability issues, e.g. flexibility and controllability, are very important for heat integrated process, since the economic performance of a process is greatly affected by process variations and the ability of the system to satisfy its operational specifications under external disturbances or inherent modeling uncertainty. During the operation, a HEN suffers disturbances in the inlet temperatures and heat capacity flow rates. These disturbances propagate through the network and may make the control of process stream target temperatures difficult if the HEN is improperly designed. In order to ensure operability issues for a designed HEN some bypasses with nominal values different of zero must be installed, and possibly the area of the bypassed heat exchanger must be increased to maintain the heat load defined in the design phase. A challenging task is to address the correct placement of the bypass and the number of bypasses to be installed once they affect the flexibility, the controllability, the operating cost and investment cost of the HEN, i.e., a 4 way tradeoff.

During the last decades, different approaches were proposed to design the control system in order to accommodate setpoint changes and to reject load disturbances in HENs. Mathisen et al. (1992) provided a heuristic method for bypass placement. Papalexandri and Pistikopoulos (1994 a, b) introduced a systematic framework for the synthesis or retrofit of a flexible and a structurally controllable HEN using a MINLP formulation. Aguilera and Marchetti (1998) developed a procedure for on-line optimization and control system design of a HEN also using a MINLP. Yan et al. (2001) proposed a model-based design for the development a retrofit HEN with optimal bypass placement using a simplified model for disturbance propagation and control.

In this work, the optimal operation and control strategy for designed heat exchanger networks are investigated and it is proposed a systematical framework where at each iteration a set of bypass candidates are selected and designed feasibly according to the minimum Operational Controllability. In section 2 the optimal operation is defined. In section 3 all components involved in the framework are described and a case study with three different designs is used as background to present the applicability of the method in section 4. Finally, some conclusions are drawn in section 5.

2 OPTIMAL OPERATION AND CONTROL OF HENS

A HEN is considered optimal operated if the targets temperatures are satisfied at steady state (main objective); the utility cost is minimized (secondary goal); and the dynamic behavior is satisfactory (Glemmestad, 1997). To ensure the requirements a control system must be design properly. It involves the control structure selection that shows good controllability according to some metric and also come along the minimization of the economic penalty, i.e with less impact on the energy cost, and on the investment cost if some area must be increased.

During the HEN operation, degrees of freedom or manipulated inputs are needed for control and optimization. The most common options are: (1) utility flowrates; (2) Bypass fraction; (3) Split fraction. Once split fractions may result in competitive effects and possible some RHP-zero, which limit the control bandwidth, only the two first options are addressed in this work. It is rather evident when a utility exchangers take place, in general as the last exchanger for each stream, they fulfill the main pairing rule, i.e. provide a fast and direct effect, with no interaction with other control loops. That is the trivial solution. Thereby, the selection of suitable sets of manipulated variables for controlling the target temperatures is a challenging problem because of its combinatorial nature. Controllability is largely dependent upon its network structure. For HENs a challenging task to be addressed is the correct placement of the bypass, i.e. the location and nominal values in order to reject disturbances.

In a HEN with n_s streams and n_u utility units, at least $n_u n_s$ extra available manipulations must be used to make the operation structurally feasible, where all target temperatures can be controlled independently. Moreover, in order to deal with positive and negative disturbances, the heat exchanger has to be designed with a steady-state flow rate for the bypass stream different than zero. For given HEN, a bypass with a specific nominal value u_{nom} can be added without changing the main HEN structure and operating point if the same heat load is maintained. Parallel to the capacity to reject disturbances ($\delta T^t = 0$), it is required an increment of the heat transfer area ($\delta A/A_0$). Therefore, a trade-off between disturbance rejection capacity and investment costs must be considered during the bypass nominal design.

A HEN shows Optimal Operational Controllability if the requirements of optimal operation are accomplished and the control objectives are fulfilled. Next section describes how to redesign a HEN for attaining Operational Controllability.

3 BYPASS DESIGN FOR OPERATIONAL CONTROLLABILITY

For a given disturbance scenario a linearized model can provide an estimation of the maximum static deviation of the system outputs. The model is embedded into a design procedure for optimality selecting bypasses that includes their location and nominal fractions. The linear model considered here is obtained from the model of each unit.

Unit Based Model – A general heat exchanger with bypass on hot and cold side is sketched in Figure 1. Based on the mass and energy balances for the heat exchanger, the mixers and splits, the model described by the set of equations from (1) to (5) can generated in a straightforward manner. The matrices (G_u, G_d^t, G_d^w), are obtained through the linearization of the model HE, using Taylor series expansion, neglecting high-order differentiation terms.

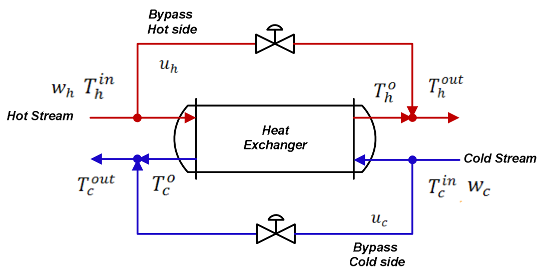

Fig. 1. General structure of a heat exchanger with bypasses.

Unit Model for the system Heat Exchanger with Bypasses.

Mixer Energy Balance:

$$\begin{bmatrix} T_h^{out} \\ T_c^{out} \end{bmatrix} = \begin{bmatrix} 1-u_h & 0 \\ 0 & 1-u_c \end{bmatrix} \begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} + \begin{bmatrix} u_h & 0 \\ 0 & u_c \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \quad (1)$$

Inner Heat Exchanger Structure:

$$\begin{bmatrix} T_h^o \\ T_c^o \end{bmatrix} = \frac{1}{(R_h' - a')} \begin{bmatrix} R_h' - 1 & 1 - a' \\ R_h'(1-a') & a'(R_h' - 1) \end{bmatrix} \begin{bmatrix} T_h^{in} \\ T_c^{in} \end{bmatrix} \quad (2)$$

Ratio between effective heat capacity flow rates:

$$R_h' \equiv \frac{(1-u_h)w_h}{(1-u_c)w_c} = \frac{T_c^o - T_c^{in}}{T_h^{in} - T_h^o} \quad (3)$$

Ratio between terminal temperature differences:

$$a' \equiv \frac{T_h^{in} - T_c^o}{T_h^o - T_c^{in}} = \exp\left(\frac{U'A}{(1-u_h)w_h} (1 - R_h') \right) \quad (4)$$

Corrected Global Heat Transfer Coefficient:

$$\frac{1}{U'} = \frac{1}{h_h(1-u_h)^{0.8}} + \frac{1}{h_c(1-u_c)^{0.8}} \quad (5)$$

The differentiation of the previous model in respect to the inlet temperatures, flowrates and bypass fractions result in the following general model for each heat exchanger:

$$\delta T^{out} = G_{u,E}\delta u + G_{d,E}^t\, \delta T^{in} + G_{d,E}^w\, \delta w \quad (6)$$

HEN Model for Disturbance Propagation and Control

If a HEN contains N_e heat exchangers, a system model can be obtained directly by lumping all unit models for a selected sequence of heat exchanger.

$$\delta T^{*out} = G_{u,E}^*\delta u^* + G_{d,E}^{*t}\, \delta T^{*in} + G_{d,E}^{*w}\, \delta w^* \quad (7)$$

The outlet and inlet temperatures flowrates of each heat exchanger is written as a function of the supply and target temperatures and flowrates of the HEN. When the stream is located in between heat exchangers called here as intermediate variables.

The temperature vectors δT^{*out} and δT^{*in} can be ordered according to the supply and target temperatures of the streams that are present in the HEN in the following manner.

$$\delta T^{in} = \left[\delta T_{H1}^s \ldots \delta T_{HN_h}^s\, \delta T_{C1}^s \ldots \delta T_{CN_c}^s\, \delta T_1^m \ldots \delta T_{N_m}^m\right]^T = [(\delta T^S)^T (\delta T^m)^T]^T \quad (8)$$

$$\delta T^{out} = \left[\delta T_{H1}^T \ldots \delta T_{HN_h}^T\, \delta T_{C1}^T \ldots \delta T_{CN_c}^T\, \delta T_1^m \ldots \delta T_{N_m}^m\right]^T = [(\delta T^T)^T (\delta T^m)^T]^T \quad (9)$$

The vector δw^* presents N_m redundant heat-capacity flow rates that should be eliminated. This reduces δw^* to $[(2N_e - N_m) \times 1]$. Correspondly,

$$G_u^* = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} = V_1 G_{u,E}^* V_4 \quad (10)$$

$$G_d^{*t} = \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} = V_1 G_{d,E}^{*t} V_2 \quad (11)$$

$$G_d^{*w} = \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} = V_1 G_{d,E}^{*w} V_3 \quad (12)$$

Where V_1 to V_4 are the conversion matrices determined by a HEN structure and bypass location. Their derivations are presented in the succeeding section. The reorganized model is equivalent to:

$$\begin{bmatrix} \delta T^T \\ \delta T^m \end{bmatrix} = \begin{bmatrix} G_{u,1} \\ G_{u,2} \end{bmatrix} \delta u + \begin{bmatrix} G_{d,11}^t & G_{d,12}^t \\ G_{d,21}^t & G_{d,22}^t \end{bmatrix} \begin{bmatrix} \delta T^S \\ \delta T^m \end{bmatrix} + \begin{bmatrix} G_{d,1}^w \\ G_{d,2}^w \end{bmatrix} \delta w \quad (13)$$

The preceding model (13) can be separated into two equations, solving the latter to the intermediate temperatures and substituting in the former yields the following model:

$$\delta T^T = G_{u,hen} \delta u + G_{d,hen}^t \delta T^S + G_{d,hen}^w \delta w \quad (14)$$

where

$$G_{u,hen} = G_{u,1} + G_{d,12}^t (I - G_{d,22}^t)^{-1} G_{u,2} \quad (15)$$

$$G_{d,hen}^t = G_{d,11}^t + G_{d,12}^t (I - G_{d,22}^t)^{-1} G_{d,21}^t \quad (16)$$

$$G_{d,hen}^w = G_{d,1}^w + G_{d,12}^t (I - G_{d,22}^t)^{-1} G_{d,2}^w \quad (17)$$

Furthermore, if the vectors of stream temperature and heat capacity flowrates are written based on classification of stream types, the model (14) can be written as

$$\begin{bmatrix} \delta T_h^T \\ \delta T_c^T \end{bmatrix} = G_{u,hen} \delta u + \begin{bmatrix} G_{d,hen,h}^t \\ G_{d,hen,c}^t \end{bmatrix}^T \begin{bmatrix} \delta T_h^S \\ \delta T_c^S \end{bmatrix} + \begin{bmatrix} G_{d,hen,h}^w \\ G_{d,hen,c}^w \end{bmatrix}^T \begin{bmatrix} \delta w_h \\ \delta w_c \end{bmatrix} \quad (18)$$

Network Structural Representation – As stated in the proceeding section, conversion matrices V_1 through V_4 are structure dependent. According to the sequence of equipment considered, the original vector of output temperatures (δT^{*out}) will present a defined order involving the target temperatures (δT^T) and the intermediate temperatures (δT^m).

<u>*Derivation of*</u> V_1. Each element of matrix V_1 has a value 0 or 1 relating the original vector δT^{*out} with the ordered vector δT^{out}. First, the matrix V_1 must have all elements set to 0. The first row of $V_1(i)$ that corresponds to the $\delta T_{h_1}^T$ relation, considering that this target is located in the k position in the disordered vector, set $V_1(i,k)$=1. It should be noted that in case of stream split, where the same temperature enters two or more heat exchangers, there will be more than one position that represent the same target. Then, in a more general way k consist in a vector of corresponding positions. The procedure must be repeated until the last row of δT^{out}.

<u>*Derivation of*</u> V_2. The matrix V_2 is generated analogously to the matrix V_1. Each element of V_2 has a value 0 or 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to $\delta T_{h_1}^S$ relation, select the k positions that this input appears in the vector δT^{*in} and for each position, set $V_2(k,j)$=1. Repeat the procedure until the last column.

<u>*Derivation of*</u> V_3. Each element of V_3 has a value between 0 and 1. The matrix must have all elements set to zero. Select the first column (j) that corresponds to δw_{h_1}relation, select the k positions that this input appears in the vector δw^* and for each position, substitute by the split fraction of the original stream flowrate, $V_3(k,j) = x_s$. Repeat the procedure until the last column.

<u>*Derivation of*</u> V_4. Each element of V_4 has a value 0 or 1. This matrix is determined by the bypass selection in a HEN, i.e. $\delta u = V_4 \delta u_{sel.}$. If it is desirable a model with all possible candidates, this matrix must be an identity matrix. In order to derive V_4, first all elements must be set to zero. Select the first column (j) that corresponds the first selected manipulated input $\delta u_{sel.}(1)$, select the k position that this input appears in the vector δu, set $V_4(k,j) = 1$. Repeat the procedure until the last column.

Bypass selection based on Controllability metrics – For regulatory purposes and the controllability of the system Kookos and Perkins (2001) proposed a mathematical programming based framework to minimize the overall interaction and sensitivity to disturbances. The resulting MILP model $(P1)$ can be used to automatic selection of the optimum set among the potential candidates.

Considering the system generally described by the transfer matrices $y = Gu + G_d d$ with the set i of outputs, set j of inputs, and set m of disturbances. The term $RGA = G \times \hat{G}^{-1}$ presenting the elements λ_{ij} can be used to calculate the $RGA\,number$ defined by (19), which is a measure of diagonal dominance pointing out the overall interaction of the pairs selected while the infinity norm of the matrix $\hat{G}^{-1}G_d$ (20) is related to the sensitivity to disturbances. For controllability purposes, both values must be as close to zero as possible. Solving the problem $(P1)$ for the weighting coefficient ρ for assigning the contribution of each term, can be used to select the best pairs according to the controllability metrics.

$$\|RGA - I\|_{sum} = \sum_{i=1}^{ny} \sum_{j=1}^{nu} \mu_{ij} \quad (19)$$

$$\|\hat{G}^{-1} G_d\|_\infty = \varphi \quad (20)$$

The parameters Ω is a sufficient large number, and $\delta_{i\ell}$ is the Kronecker delta (i.e. 1 if $i = l$, 0 otherwise) and g_{ij} and $g_{d,im}$ the elements of G and G_d respectively. The additional symbols represent auxiliary variables used to compute (19) and (20). The decision variables X_{ij} represent the binary variables that assume value 1 if j is selected to control i, and 0 otherwise.

$$
\left\{
\begin{array}{l}
min \quad J_1 = \rho\varphi + (1-\rho)\sum_{i=1}^{ny}\sum_{j=1}^{nu}\mu_{ij} \\
\qquad \sum_{i=1}^{ny} X_{ij} - 1 \le 0 \\
\qquad \sum_{j=1}^{nu} X_{ij} - 1 = 0 \\
\sum_{i=1}^{nu} g_{ij}\,\tilde{g}_{\ell j} - \delta_{i\ell} = 0, \qquad \forall\, i, \ell \\
\left.\left\{
\begin{array}{c}
-\Omega\sum_{i=1}^{ny} X_{ij} \le \tilde{g}_{\ell j} \le \Omega\sum_{i=1}^{ny} X_{ij} \\
\lambda_{ij} - g_{ij}\tilde{g}_{ij} = 0 \\
\eta_{ij} = \lambda_{ij} - X_{ij} \\
-\mu_{ij} \le \eta_{ij} \le \mu_{ij}
\end{array}
\right.\right\} \forall\, i, j \\
\sum_{i=1}^{ny} \tilde{g}_{ij} g_{d,im} - \sigma_{jm} = 0, \qquad \forall\, j, m \\
\quad \left.\left\{
\begin{array}{c}
-\epsilon_j \le \sum_{m=1}^{nd} \sigma_{jm} \le \epsilon_j \\
\epsilon_j - \varphi \le 0
\end{array}
\right.\right\} \forall\, j, m \\
X_{ij} = \{0,1\}, \quad \mu_{ij} \ge 0, \qquad \epsilon_j \ge 0 \;\; \forall\, i, j
\end{array}
\right\} \quad (P1)
$$

Priority Matrix – The application of the model $P1$ can ensure the optimal pair set according to the criteria selected. However its application to HENs requires some additional details in order to ensure the optimal operation.

Feasibility: in order to deal with positive and negative disturbances, the heat exchanger has to be designed with a steady-state flow rate for the bypass stream different than zero. But besides the opportunity to reject disturbances $(\delta T^t = 0)$, its installation must cause an increment of the heat transfer area $(\delta A/A_0)$. The designer must be aware that the optimal nominal fraction is the lowest value able to provide the total disturbance rejection.

Economic Penalty: different bypasses selection can affect the utility cost in different ways. Therefore the emerging question is how to select the best pairs taking into account that information. The priority matrix proposed by Glemmestad (1997) is used to address this issue.

We can consider the bypass controlled outputs, and the corresponding inner system that has an upstream utility exchanger. Considering the energy balance on the utility exchangers it is possible to put the heat utility loads as a function of bypass fractions:

$$
\begin{bmatrix} \delta T_h^o \\ \delta T_c^o \end{bmatrix} = G_{bp}\delta u; \quad \begin{bmatrix} \delta Q_{HU} \\ \delta Q_{CU} \end{bmatrix} = G_q \delta u \tag{21}
$$

The vector of cost associated with the hot and cold utilities c^T yields $g^{U\$} = cG_q$, which give us the information about how the manipulation of the bypass fractions impacts on the utility cost. Introducing the control error subject to a given output i, e_i, we can define a "priority matrix" P that whose element p_{ij} is the cost to bring the outputs back to its target value.

$$
p_{ij} = -\frac{g_j^{U\$}}{G_{bp,ij}} e_i \tag{22}
$$

The matrix P consists of as many rows as there are controlled temperatures and as many columns as there are inputs that may be manipulated. Therefore, the pairing that results in minimum total utility cost according to P should be selected.

Worst Cases Scenarios – To estimate the priority matrix elements and estimate the bypass nominal value able to reject the disturbances, the errors e must be known. According to Yang et. al (2001) the worst cases form the bypass nominal value point of view based on the constant sign of disturbance propagation in HENs can be defined by the following equations, where the superscript $(+)$ and $(-)$ point out the positive and negative deviations:

$$
\begin{aligned}
e^+ &= \delta T_d^{t(+)} \\
&= G_d^{t^h}\delta T^{s(+)^h} + G_d^{t^c}\delta T^{s(+)^c} + G_d^{w^h}\delta w^{(+)^h} \\
&- G_d^{w^c}\delta w^{(-)^c}
\end{aligned} \tag{23}
$$

$$
\begin{aligned}
e^- &= \delta T_d^{t(-)} \\
&= G_d^{t^h}\delta T^{s(-)^h} + G_d^{t^c}\delta T^{s(-)^c} + G_d^{w^h}\delta w^{(-)^h} \\
&- G_d^{w^c}\delta w^{(+)^c}
\end{aligned} \tag{24}
$$

And it is determined the necessary control correction vectors to each case

Nominal Value Estimation – Assuming perfect control for each scenario $(+)$ and $(-)$ and a subset of manipulated variables (δu_s) the bypass fractions need to reject the disturbance loads are $\delta u_s{}^{(+)}/\delta u_s{}^{(-)}$, calculated by solving the optimization problem $(min \;\; \|G_u V_4 \delta u_s + e\|_2)$ using e^+ and e^- respectively. According to the minimum economic penalty the decision must be made according to the equation, and the nominal values is updated according to

$$
u_{new} = -min\{\delta u_s{}^{(+)}, \delta u_s{}^{(-)}\} \tag{25}
$$

In addition for each bypass selected and designed, we must ensure no violation of the upper permissible nominal value given by the equations.

For bypass on hot side:

$$
u_{lim}^k = \frac{T_h^{out,k} - T_c^{in,k} - \Delta T_{min}}{T_h^{in,k} - T_c^{in,k} - \Delta T_{min}} \tag{26}
$$

For bypass on cold side:

$$
u_{lim}^k = \frac{T_h^{in,k} - T_c^{out,k} - \Delta T_{min}}{T_h^{in,k} - T_c^{in,k} - \Delta T_{min}} \tag{27}
$$

The feasibility (areas non infinity) is ensured holding the following constraint:

$$|\delta u_s^{(-),k}| + |\delta u_s^{(\mp),k}| \le u_{lim}^k \quad (28)$$

Also a heuristic constraint is added to avoid bypass both sides of the same heat exchanger, which yields singularity. The resulting model $P2$ is described as follows:

$(P2)$ ***Optimal Pairing Selection:*** *(For economic penalty)*

Minimum Utility Consumption (optimal pairing)

$$\min_{X} \sum_{i=1}^{ny}\sum_{j=1}^{nu} p_{ij}^{+} X_{ij} + \sum_{i=1}^{ny}\sum_{j=1}^{nu} p_{ij}^{-} X_{ij}$$

One bypass pr. bypass controlled temperature

$$\sum_{i=1}^{ny} X_{ij} - 1 \le 0$$

Each bypass can not control more than one output.

$$\sum_{j=1}^{nu} X_{ij} - 1 = 0$$

Reject pairs when $G_{bp,ij} = 0$

$$X_{ij} + g_{ij}^{0} \le 1$$

One degree of freedom per Heat Exchanger

$$\sum_{i=1}^{ny} X_{ij} + \sum_{i=1}^{ny} X_{ij' \neq j} \le 1$$

Avoiding violation of the upper permissible value

$$\left|\delta u_{hE_i}^{+}\right| + \left|\delta u_{hE_i}^{-}\right| \le u_{hE_i}^{lim} X_{ij}$$

$$\left|\delta u_{cE_i}^{+}\right| + \left|\delta u_{cE_i}^{-}\right| \le u_{cE_i}^{lim} X_{ij}$$

Model for Optimal Operational Controllability – Combining the model $(P1)$ and $(P2)$, summing up the objective functions and the two set of constraints result in the complete model for optimal operational controllability. It should be noted that the procedure result in a $MILP$ $(P3)$, which provides the bypass allocation, the nominal values with minimum economic penalty and the controllability metrics.

Optimal Bypass Design – Initialize the bypass nominal values (normally zero for the classic designs methods), the model for disturbance propagation is obtained and the problem (P3) is solved to ensure optimal operational controllability. The model is retrofitted updating the matrices G_u, G_d^t, and G_d^w with the selected nominal bypasses values and all the procedure is repeated until the convergence. The convergence is checked ($|\delta u_{new} - \delta u_{old}| \le \varepsilon$), where ε is the permissible computational error. At the end the new areas of heat exchangers bypassed are estimated (the tradeoff is implicitly considered by the $\Delta T_{\min}$ used in the equations (26) and (27)) and the model is used to calculate stream outputs deviations and the utility consumption is estimated to the worst case design. The new Total Annual Cost is estimated, the best solution is that with the lowest TAC.

Dynamic Modeling – The different retrofitted HENs can be compared in terms of dynamic performance. The dynamic model is obtained modeling N cells according to the equations (29) and (30). The same procedure used to obtain the static model of the system can be used to derive the system dynamic model.

$$\rho_h V_h^i Cp_h \frac{dT_h^i}{dt} = \dot{m}_h Cp_h \left(T_h^{i-1} - T_h^i\right) - UA^i \Delta T_{ef}^i \quad (29)$$

$$\rho_c V_c^i Cp_c \frac{dT_c^i}{dt} = \dot{m}_c Cp_c \left(T_c^{i+1} - T_c^i\right) + UA^i \Delta T_{ef}^i \quad (30)$$

4 CASE STUDY

In this section 3 different HENs depicted in Fig. 2 are used as background. Table 1 list the design data and the disturbance information need to compute the worst case design.

Table 1. Design data for the Case Study.

Stream	T^t (ºC)	T^s (ºC)	F (kWºC^{-1})	h (kW m^2 ºC^{-1})
H1	270	160	18	1
H2	220	60	22	1
C1	50	210	20	1
C2	160	210	50	1
CU	15	20		1
HU	250	250		1

Cost of Cooling Utility = 20 (\$kW^{-1}y^{-1})
Cost of Heating Utility = 200 (\$kW^{-1}y^{-1})
$\delta T^{(+)} = \delta T^{(-)} = 2$ *and* $\delta w^{(+)} = \delta w^{(-)} = 10\%$

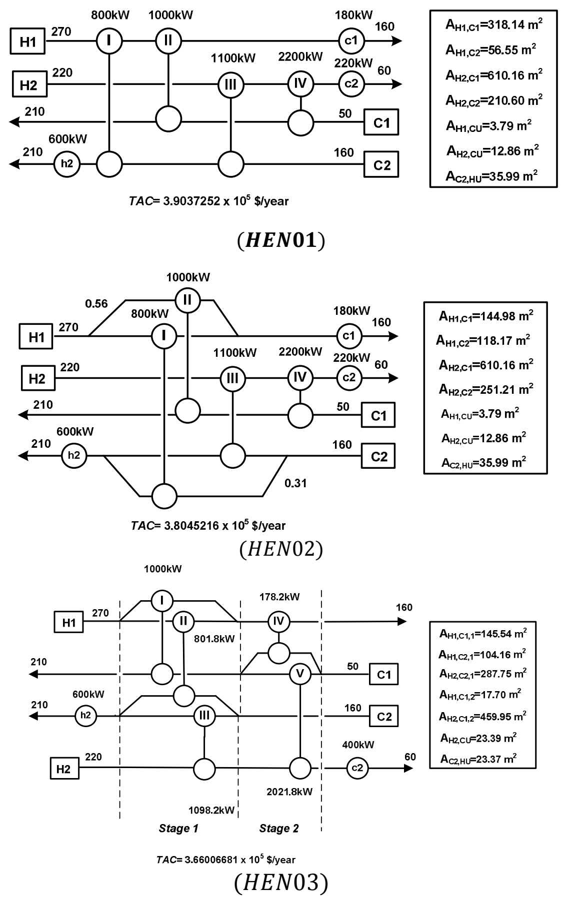

Fig. 2. HENs Designed for the Case Study u for $\Delta T_{min} = 10$ using different approaches.

For each HEN it was considered the outlet temperatures as controlled variables $\delta T^t = [\delta T_{h1}^t \quad \delta T_{h2}^t \quad \delta T_{c1}^t \quad \delta T_{c2}^t]^T$ and as potential candidates for the bypass controlled targets $\delta u = \left[u_{1,1}^h \quad u_{1,1}^c \quad u_{1,2}^h \quad u_{1,2}^c \quad u_{2,1}^h \quad u_{2,1}^c \quad u_{2,2}^h \quad u_{2,2}^c\right]^T$ for the first HEN and amorously for the others. To ensure the structural feasible operation the maximum number of bypasses was installed. The model was solved with $\rho = 0.5$, $M = 100$. The results are summarized in the Table 2.

Table 2. Bypass Nominal Design for the 3 structures.

hen	*y set*	*u set*	*Nom. Values*	*RGA Number*	$(\delta A/A_0)$ %	*TAC ($/y)*
	T_{h2}^t	$u_{2,1}^h$	0.0296		20.93	
01	T_{c1}^t	$u_{1,1}^c$	0.0748	0	10.85	409,294
	T_{c2}^t	$u_{2,2}^c$	0.1024		9.03	
	T_{h2}^t	$u_{2.1}^h$	0.0258		9.29	
02	T_{c1}^t	$u_{1.1}^h$	0.1604	0	18.32	399,550
	T_{c2}^t	$u_{1,2}^c$	0.1926		19.23	
	T_{h1}^t	$u_{1,2,1}^c$	0.0491		3.92	
03	T_{c1}^t	$u_{2.1.2}^h$	0.0800	1.44	25.27	392,782
	T_{c2}^t	$u_{2.2.1}^h$	0.0563		18.69	

One target temperature is controlled using the utility flowrate, it was selected to manipulate the cheaper utility. The results show that different investment levels are needed to each case, since the structure limits the operability as expected. Comparing the three HENs the last one needs more investment, but the previous costs associated with the critical consumption assumed by the utility controlled target (considered to estimate the operating cost) still result in the cheaper solution.

This procedure must reject non controllable HENs, and provide a decision based on the trade-off between controllability and total costs, i.e. the optimal operational controllability. It should be noted that the third structure represent the cheaper solution but the interaction as pointed out by the RGA number was larger. Even tough, the HEN03 presented the best operational controllability. For a final decision, and fulfillment of the third goal in optimal operation of HENs the dynamic model must be analyzed.

In Figure 3, is verified the convergence behavior running the iterative design for the solution shown in Table 2 for the $HEN01$. For a tolerance of 10^{-4} the solution converges after 6 iterations with 3.06 seconds. Increasing the disturbance data by 50% the convergence is achieved with more iterations and 9.32 seconds are needed.

5 CONCLUSIONS

The bypass design for HENs was accomplished through optimal operation problem taking into account the trade-offs between energy cost, investment cost and the controllability in order to ensure an economic operation. The design of a HEN cost effective capable to be controlled has both economical and operational significance. The controllability depends on the HEN structure, but to be evaluated in fact it is not necessary to design the controller, but it must be selected a set of manipulated and controlled variables. It was presented a systematic framework model-based to design an appropriated control system, selecting the manipulated set, and design bypasses with minimum economic penalty. Through the prediction of the disturbances on controlled variables, it is possible to estimate the bypasses nominal fractions able to reject these disturbances solving an analytical problem per iteration resulting in a fast and robust procedure. The results demonstrate that the 3 structures analyzed are high controllable with similar total annual cost. In order to make a final decision a comparative controllability analysis including the dynamic performance should be performed.

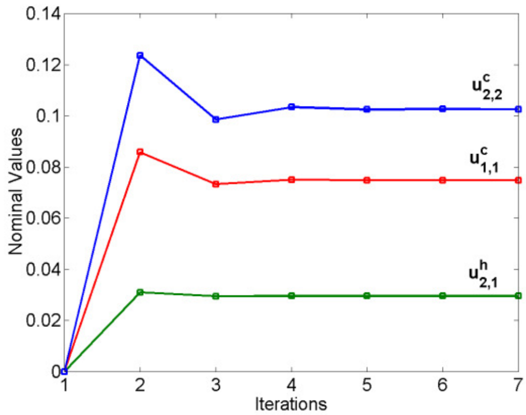

Fig. 3. Iterative Bypass design for $HEN01$ with, T_{h2}^t, T_{c1}^t, T_{c2}^t as bypass controlled.

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Appendix C

Optimization Overview

Optimization has become a major enabling area in process systems engineering. It that has evolved from a methodology of academic interest into a technology that has and continues to make significant impact in industry (Biegler and Grossmann, 2002). Mathematical Programming, and optimization in general, have found extensive use in process systems engineering. The main applications, design and synthesis, operations and control, have been facilitated not only by progress in optimization algorithms, but also by the advent of modeling techniques (Williams, 1985) and modeling systems such as GAMS (Brooke et. al, 1998), AMPL (Fourer et al., 1992) and LINDO (Schrage, 1997). Most modeling systems support a variety of solvers, while the more popular codes can be used with many different modeling systems. A solver is concerned primarily with solving individual mathematical programs. Solvers are thus distinguished by the algorithms they implement, and by the mathematical categories of optimization problems for which they are able to find optimal solutions. A general overview can be found in the Figure 1, where is presented the main classes of mathematical problem, the main general algorithms for each problem type, the main solvers packages and modeling systems with their respective interfaces. There is no universal optimizer that is well suited to any kind of optimization problem whatsoever. The selection of a flexible modeling system (Table 1) as well as the selection of suitable solvers (Table 2) by which a generated model can be solved is often a critical issue in obtaining valuable results in modeling applications.

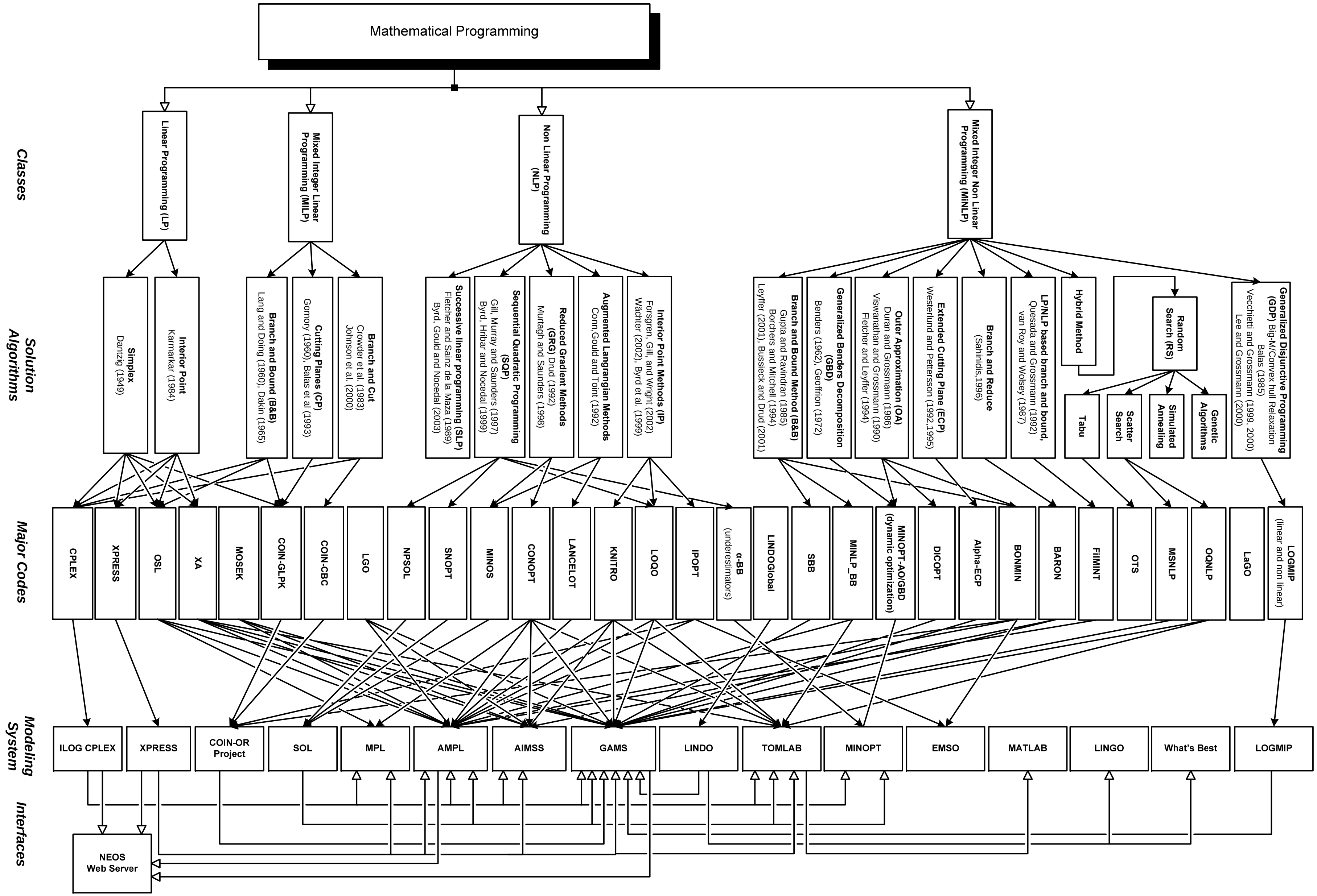

FIGURE C.1: OVERVIEW OF OPTIMIZATION TOOLS.

TABLE C.1: MODELING LANGUAGES AND SYSTEMS FOR OPTIMIZATION.

High Level System	Latest Version	Developer	Main World Class Solvers
GAMS General Algebraic Modeling System	22.8	GAMS Development Corporation http://www.gams.com/	LP, NLP, MIP, MILP, MINLP. AlphaECP, BARON, BDMLP, Coin-Cbc, Coin-Glpk, CONOPT, CPLEX, DECIS, DICOPT, KNITRO, LINGO, LGO, LINDOGlobal, MINOS, MOSEK OSL, SBB, SNOPT, XA, XPRESS.
AMPL A Modeling Language for Mathematical Programming	2nd ed.	Bell Laboratories http://www.ampl.com/	LP, NLP, MIP, MILP, MINLP. Bonmin, Coin-Cbc, CONOPT, CPLEX, IPOPT, KNITRO, LANCELOT, LGO, LOQO, MINLP_BB, MINOS, MOSEK, NPSOL, NETSOL, OSL, SNOPT, XA, XPRESS.
AIMSS Advanced Interactive Multi-Dimensional Modeling Software	3.8	Paragon Decision Technology http://www.aimms.com/	LP, NLP, MIP, MILP, MINLP. BARON, CONOPT, CPLEX, KNITRO, LGO, MINOS, MOSEK, NPSOL, OA, SNOPT, XA, XPRESS.
BARON Branch and Reduce Optimization Navigator	4.0	Dept. of Chem. Eng. University of Illinois http://archimedes.cheme.cmu.edu/baron/	MILP, MIQP, NLP, MINLP, Global (Linear and Nonlinear) BARON.
ILOG CPLEX	11.1	ILOG Inc. http://www.ilog.com/	LP, QP, MILP, MIQP. ILOG CPLEX- Simplex, Barrier and Mixed Integer Optimizer.
LINGO Modeling Environment and Solver	11.0	LINDO Systems Inc. http://www.lindo.com/	LP, Integer Programming, QP, NLP, MILP, MINLP, Global. Simplex, Barrier, Integer, GRG, SLP.
LINDO API Premier Optimization Engine	5.0	LINDO Systems Inc. http://www.lindo.com/	LP, QP, NLP, MILP, MINLP, Global. Simplex, Barrier, Integer, GRG, SLP, LINDOGlobal.
MPL Mathematical Programming Language	4.2	Maximal Software Inc. http://www.maximal-usa.com/	LP, QP, NLP. CONOPT, CPLEX, LSGRG2, OSL, XPRESS.
What'sBest The Spreadsheet Solver	9.0	LINDO Systems Inc. http://www.lindo.com/	Add-in to Excel LP,MILP,MINLP, NLP.
MATLAB	2008a	Mathworks Inc. http://www.mathworks.com/	LP, NLP, QP, Multiobjective. **Uncostrained:** Quasi-Newton (BFGS), Nelder-Mead (Direct Search), and trust-region. **Conctrained:** trust-region, active-set SQP, and interior-point.IP, Simplex, B&B.
MINOPT A Modeling Language and Algorithmic Framework	3.1	Dept. of Chem. Eng., Princeton University. http://titan.princeton.edu/MINOPT/	LP, NLP, NLP/DAE, MIP, MILP, MINLP/DAE, OCP, MIOCP. CPLEX, LPSOLVE, MINOS, NPSOL, SNOPT, DASOLV, DAESSA. MINLP: GBD, OA, OA/ER, OA/ER/AP, GCD.
TOMLAB A General Purpose MATLAB Environment for Optimization	v6.1	Kenneth Holmström, TOMLAB Optimization http://tomopt.com/tomlab/	Toolbox to Matlab: LP, MILP, NLP, MINLP. CPLEX, CONOPT, KNITRO, LGO, LOQO,MINLP, MINOS, NPSOL, NPOPT, NLSSOL, OQNLP, QPOPT, SNOPT, XA, XPRESS.
EMSO Environment for Modeling, Simulation, and Optimization	0.9.57	Dept. of Chem. Eng., UFRGS. http://www.enq.ufrgs.br/trac/alsoc/wiki/EMSO	LP, NLP, MINLP. Bonmin, IPOPT.
XPRESS-MP	2008A	Dash Associates Ltd. http://www.dashoptimization.com/	LP, QP, NLP, MILP, MIQP, MINLP. XPRESS-SLP, SP, Mosel, BCL, Kalis.
NEOS Server Web-based access to AMPL, GAMS, and many other solvers.	4.0	Argonne National Laboratory http://www-neos.mcs.anl.gov/	LP, MIP, MILP, NLP, MINLP. CPLEX, CONOPT, GRG2, KNITRO, LANCELOT, LGO, LINDO, LINGO, LOQO, LSGRG2, MINOS, MOSEK, NPSOL, NPOPT, NLSSOL, OML, OQNLP, OSL, QPOPT, SNOPT, XA, XPRESS.
SOL/UCSD Systems Optimization Laboratory	2008	Stanford Business Software Inc. http://www.sbsi-sol-optimize.com/	Portable Fortran 77 source code for LP, QP, NLP. Simplex, MINOS, LSSOL, NPSOL, QPOPT, SQOPT, SNOPT.

TABLE C.2: MAIN SOFTWARES/SOLVERS FOR OPTIMIZATION.

Software	Latest Version	Capability	Algorithm Type	Developer/Reference
CPLEX	11.0	LP, MILP	Simplex, Interior Point (IP), Branch and Bound (B&B)	ILOG CPLEX. (ILOG, 2003)
XPRESS	18.0	LP, MILP	Simplex, Interior Point (IP), Branch and Bound (B&B)	Dash Associates. (Dash Associates, 1999)
OSL	2.0	LP, MILP	Simplex, Interior Point (IP), Branch and Bound (B&B)	IBM Corporation. (Wilson, 1992)
XA	13.97	LP, MILP	Simplex, Interior Point (IP), Branch and Bound (B&B)	Sunset Software Technology. (XA, 2004)
MOSEK	5.0	LP, MILP	Simplex, IP, Branch and Bound and Cut	MOSEK ApS. (MOSEK, 2008)
Coin-Cbc	2.2	LP, MILP	Simplex, Branch and Cut	John Forrest, IBM. COIN-OR (Forrest and Lougee-Heimer, 2004)
Coin-Glpk	4.8	LP, MILP	Simplex, Interior Point (IP), Branch and Bound (B&B)	Moscow Aviation Institute. COIN-OR (Makhorin, 2004)
CONOPT	3.10	NLP	Generalized Reduced Gradient (GRG) Method	ARKI Consulting & Development A/S. (Drud, 1992)
MINOS	5.5	NLP	Simplex, Reduced Gradient, Augmented Lagrangian	Stanford Business Software, Inc. (Murtagh and Saunders, 1998)
KNITRO	5.2	NLP	Interior Point Method, Trust Region	Ziena Optimization Inc. (Byrd, et al., 1999)
SNOPT	7.0	NLP	Sparse Sequential Quadratic Programming (SQP)	Stanford Business Software, Inc. (Gill et al.,1997)
IPOPT	3.5.1	NLP	Interior Point Filter Line Search	COIN-OR Project. (Wächter and Biegler, 2006)
LOQO	6.07	NLP	Interior Point Line Search	Princeton University (Vanderbei, 1994)
NPSOL	5.0	NLP	Active set, Line search, dense SQP	Stanford Business Software, Inc. (Gill et al.,1986)
LANCELOT	A	NLP	Augmented Lagrangian	Conn A., Gould N. and Toint P. (Conn et al., 1992)
AlphaECP	5.101	MINLP	Extended Cutting Plane (ECP)	Åbo Akademi University. (Westerlund and Pettersson, 1995)
DICOPT	2x-c	MINLP	Outer Approximation (OA)	Carnegie Mellon University. (Viswanathan and Grossmann, 1990)
MINOPT-OA	3.1	MINLP	Outer Approximation (OA)	Princeton University. (Schweiger and Floudas , 1998)
MINOPT-GBD	3.1	MINLP	General Benders Decomposition (GBD)	Princeton University. (Schweiger and Floudas , 1998)
Bonmin	0.99.3	MINLP	Branch & Bound, Branch &Cut, Outer Approximation	CMU/IBM. COIN-OR (Bonami et al., 2005)
MINLP BB	-	MINLP	Branch and Bound with SQP	Argonne National Laboratory. (Leyffer, 2001)
SBB	1.0	MINLP	Standard B&B and any NLP solver supported	ARKI Consulting & Development A/S. (Bussieck and Drud, 2001)
LOGMIP	1.0	MILP,MINLP	GDP-Big M/ Convex Hull Relaxations, OA	Ingar/ Carnegie Mellon Univ. (Vecchietti and Grossmann, 1999)
OQNLP	-	MINLP, NLP, GO	Multi Start Scatter Search and any NLP solver	Optimal Methods, Inc. /OptTek Systems, Inc.(Ugray et al. , 2003)
AlphaBB	-	NLP, GO	Branch & Bound, Convex Underestimators	Princeton University. (Adjiman et al. , 1996)
LGO	4.0	NLP, GO	Lipschitz-constraints, Adaptative Randon Search	Pinter Consulting Services, Inc. (Pintér, 1997)
LINDOGlobal	5.0.1.274	MINLP, GO	Branch & Cut Method	Lindo Systems, Inc. (Schrage ,1991)
BARON	8.1.5	MINLP, NLP, GO	Branch and Bound + Range Reduce.	University of Illinois at Urbana Champaign. (Sahinidis, 1996)
LaGO	0.3	MINLP, GO	Heuristic Branch and Cut	Humboldt Univ. of Berlin. COIN-OR (Nowak et al, 2003)

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