EFFICIENCY EVALUATION OF VALVE TRAYS WITH DOWNCOMER AND DUALFLOW TRAYS OF INDUSTRIAL DISTILLATION COLUMNS

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Abstract. The main objective of this work is to establish appropriated ways for estimating the efficiencies of valve trays with downcomer and dualflow trays of industrial distillation columns. The knowledge of efficiencies has fundamental importance in the design and performance evaluation of distillation columns. Searching in the literature, a tree of alternatives was identified to compose the tray efficiency model, depending on the mass transfer models, the liquid distribution and vapor flow model on the tray, the liquid drag model, the multi-component mixture equilibrium model, the physical properties models, the height of froth on the tray model and the efficiency definition. In this work, different methods to predict the efficiency in valve trays and dualflow trays were composed and compared against data from three industrial distillation columns under different operating conditions. The models were inserted in the Aspen Plus 12.1 simulator, in Fortran language, together with geometrical tray data, fluid properties and operating data of the distillation columns. For each column the best thermodynamic package was chosen by checking the temperature profile and overhead and bottom compositions obtained via simulation against the corresponding actual data of industrial columns. A modification in the parameter representing the fraction of holes in jetting, in the hydraulic model of the dispersion above the tray from Garcia (1999), was proposed. Modification produced better results in the prediction of the fraction of holes in jetting and efficiency in dualflow trays and similar results to Garcia (1999) to the efficiency in valve trays.

Keywords: Fractionated distillation, Tray efficiency, Distillation columns

1. Introduction

In the petrochemical industry, tray column is one of the most utilized equipment in the separation of liquid mixtures and vapor/gas mixtures (Xu et al., 1994). Trays are rated in two types, according to their flow characteristics: crossed-flow and counter-current.

In trays with crossed flow, the liquid flows between the trays through the downcomers, and the vapor flows only through holes, valves or bubble caps. Much less known, the dualflow trays are those where the counter-current flows of liquid and vapor pass through the same holes, do not downcomers and may present a waved profile. These trays have a higher capacity and present a lower pressure drop than those trays with downcomers, since the flow occurs through the whole cross-sectional area of the column (Xu et al., 1994). Such trays also provide a reasonable mass transfer with a low amount of investment. They are used for those applications where there is presence of solids and polymers (Garcia and Fair, 2002). Despite the more frequent use of dualflow trays in the petrochemical and oil industries, publications related to the efficiency estimation of such trays are considered as being rare. According to Garcia and Fair (2002), more and more crossed-flow trays are being replaced by dualflow trays aiming at solving those problems caused by severe particle deposits.

Presently, a continuously reducing number of data and methods developed for efficiency estimation are

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being published by those who detain tray-manufacturing technology. Furthermore, existing methods are still relatively inaccurate (Klemola and Ilme, 1996).

Garcia (1999) / Garcia and Fair (2000) have presented a fundamental theoretical model devised for estimating tray efficiency with downcomer. Such model was an improvement, designed to be used in organic systems, of the model suggested by Prado and Fair (1990), for air/water systems, which divided the tray into zones and applied to each one of such zones the two-layer mass transfer theory and the type of hydraulic regime. Prado and Fair (1990) took into consideration three regions: the one close to the holes, where the gas may be under either a jetting or bubbling condition; the bulk froth region, which is composed by gas bubbles dispersed through the liquid, and the spray zone. Until then, the correlation established by Chan and Fair (1984) was the one developed using more data and the one more recommended in publications for the use with valve trays (Bennett et al., 1997).

Garcia and Fair (2002) amplified the application of the zones model devised by (1999) / Garcia and Fair (2000) for *dualflow* trays. Up to this moment, the most recent attempt of modeling the efficiency of this tray type had been made by Xu et al. (1994).

The main goal of this work was to implement, in the Aspen Plus 12.1 simulator, the equation sequence and correlations between those methods by Garcia (1999) / Garcia and Fair (2000); Xu et al. (1994), and Chan and Fair (1984) for the prediction of overall efficiency of columns with dualfow trays and valve trays with downcomer, making the data available for industrial use and comparing the overall efficiency results of such models with overall efficiency from industrial columns. In addition, a modification was suggested to the *FJ* parameter (fraction of holes in *jetting*) in the model by Garcia (1999). At the end, a verification was made as to which is the best method to be used according to the tray type.

2. Model Development

This section presents the theorical model proposed by Prado and Fair (1990) and improved by Garcia (1999) / Garcia and Fair (2000), which in the next section is compared to the model by Chan and Fair (1984) for valve trays with downcomer, and to the model by Xu et al*.* (1994) for dualflow trays. Furthermore, as suggested in this work, the modification in the calculation of fraction of holes in jetting from the model by Garcia (1999) / Garcia and Fair (2000) is also presented.

2.1. Model Structure

The modeling suggested by Prado and Fair (1990) for water /air systems, and improved by Garcia (1999) / Garcia and Fair (2000) for organic systems, divides the tray into six zones, as shown in Figure 1. At any given moment, zones are characterized by one of the types of vapor flow dispersion: jet, large bubbles and small bubbles. The size of each of these zones varies according to the volumetric flow rate of liquid and vapor.

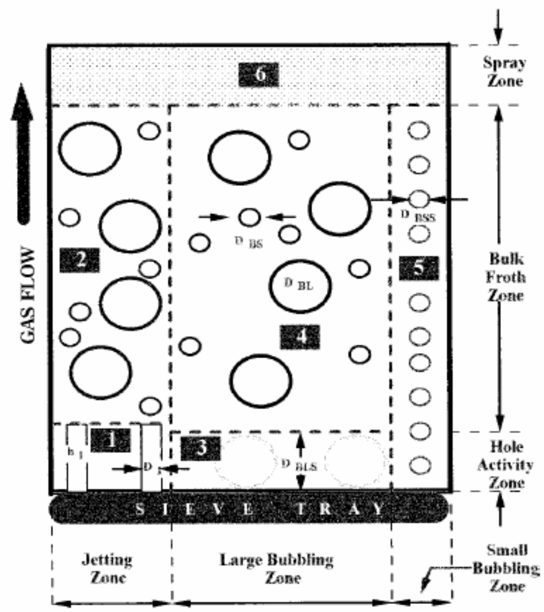

Fig. 1. Hydraulic dispersion model above the tray (Prado and Fair, 1990).

Each zone is separately modeled in terms of number of mass transfer units in the gas and liquid phases (N_G e N_L). Each zone's contribution for the prediction of point efficiency (E_{OG}) by tray is obtained by means of Eq. 1, where N_{GFJ} and N_{GFLB} are obtained through Eq. 2 and 3, respectively:

$$E_{OG} = FJ.(1-e^{-N_{GFJ}}) + FLB.(1-e^{-N_{GFLB}}) + FSB.(1-e^{-N_{G5}}) \quad (1)$$

$$N_{GFJ} = N_{G1} - ln\{1-[AJ.(1-e^{-N_{G2S}}) + (1-AJ).(1-e^{-N_{G2L}})]\} \quad (2)$$

$$N_{GFLB} = N_{G3} - ln\{1-[AJ.(1-e^{-N_{G4S}}) + (1-AJ).(1-e^{-N_{G4L}})]\} \quad (3)$$

The correlation for estimating *FSB* is obtained from Eq. 4, *FJ* from Eqs. 5 and 6, and *FLB* from Eq. 7.

$$FSB = 165,65.d_H^{1,32}.\phi^{1,33} \quad (4)$$

$$FJ_{modified} = \frac{u_A.0,60}{u_{AT}} \quad (5)$$

$$u_{AT} = 0,04302.\rho_G^{-0,5}.\rho_L^{0,692}.\sigma^{0,06}.\phi^{0,25}.\left(\frac{Q_L}{L_W}\right)^{0,05}.d_H^{-0,1} \quad (6)$$

$$FLB = 1 - FJ - FSB \tag{7}$$

The original correlation suggested by Prado and Fair (1990) for the calculation of *FJ*, which was used by Garcia (1999) / Garcia and Fair (2000), is shown in Eq. 8. Prado and Fair (1990) compared the superficial gas velocity (u_A) based in the active area with empirical correlations for the calculation of minimal and maximum jet velocity (Eqs. 9 and 10).

$$FJ = \frac{u_A - u_{A,0}}{u_{A,100} - u_{A,0}} \qquad 0 < FJ < 1 \tag{8}$$

where $u_{A,0}$ is the superficial gas velocity, based on the active area, with 0 % of *jetting*, and $u_{A,100}$ is the superficial gas velocity, based on he active area, with 100 % of *jetting*, calculated through Eqs. 9 and 10:

$$u_{A,0} = 0{,}1.\rho_G^{-0,5}.\rho_L^{0,692}.h_W^{0,132}.d_H^{-0,26}.\phi^{0,992}.\left(\frac{Q_L}{L_W}\right)^{0,27} \tag{9}$$

$$u_{A,100} = 1{,}1.\rho_G^{-0,5}.\rho_L^{0,692}.h_W^{0,132}.d_H^{-0,26}.\phi^{0,992}.\left(\frac{Q_L}{L_W}\right)^{0,27} \tag{10}$$

The Eq. 5 showed above is the modification in the *FJ* calculation suggested by this work for the model presented by Garcia (1999) / Garcia and Fair (2000), based upon the statement made by Johnson (apud Prado et al., 1987) that 60 % of the tray holes are under the jet condition when the superficial gas velocity based on the active area in the transition point from the froth condition to the *spray* condition (u_{AT}) is reached. The correlation for the u_{AT} calculation was presented by Johnson (apud Prado et al., 1987), showed in Eq. 6.

The models for the calculation of N_G and N'_L in each one of the zones are based upon the two-film theory: $N_G = k'_G.a'.t_G$ and $N'_L = k'_L.\bar{a}.t_L$.

Residence times are calculated through the velocities of *jet*, ascendance of bubbles and by the liquid height over the tray (h_F). For the h_F calculation on waved trays, the Garcia and Fair (2002) correlations were used; on the valve trays, the Dhulesia (apud Lockett, 1986) and Todd and Van Winkle (apud Lockett, 1986) correlations were used.

2.2. Mixture Models

Once the point efficiency by tray (E_{OG}) is obtained, it is necessary to relate it to the Murphree tray efficiency (E_{MV}). The simulator utilizes the Murphree tray efficiency in the gas phase for the calculation of the column. In dualflow trays, (counter-current flow), the point efficiency is the same as the Murphree tray efficiency, that is, *Pe* is zero. For the valve trays, the mixture model developed by Lewis was used, which is recommended by Lockett (1986), and is given by Eq. 11, if $Pe \geq 20$ (*plug flow*), or by Eq. 12, if $Pe < 20$ (partial mixture).

$$E_{MV} = \frac{(e^{\lambda . E_{OG}} - 1)}{\lambda} \tag{11}$$

$$\frac{E_{MV}}{E_{OG}} = \frac{1 - [e^{-(\eta + Pe)}]}{(\eta + Pe).\left[1 + \frac{(\eta + Pe)}{\eta}\right]} + \frac{e^{\eta} - 1}{\eta.\left[1 + \frac{\eta}{(\eta + Pe)}\right]} \tag{12}$$

In a multi-component system, the phase equilibrium curves are different for each component. The pseudo-binary method was used for the calculation of *m*, where the composition of the light and heavy key-components in the liquid and vapor phases was taken into consideration (Lockett, 1986).

2.3. Liquid Entrainment and Weeping

The liquid entrainment by the vapor to the top tray reduces the column efficiency, due to the fact that it is an internal recirculation of the liquid. For dualflow trays, the correlation suggested by Garcia and Fair (2002) was used, while the correlations suggested by Colburn (apud Lockett, 1986) and Zuiderweg (1982) were used for valve trays, in order to consider the effect produced by such drag.

In relation to weeping, the correlation suggested by Garcia (2002) was used for dualflow trays, while for valve trays the effect of weeping in the tray efficiency was not considered, because "[...] there is not an equation that is conveniently simple and analogous to the one suggested by Colburn (1936), designed to determine the apparent efficiency under weeping conditions" (LOCKETT, 1986, p. 175). In this work, only the weeping flow rate was determined, which is expected to be well below, or even non-existent, in the case of valve trays.

3. Methodology

3.1. Evaluated Distillation Columns

The columns specifications are showed in Table 1. The three distillation columns utilized as reference for this study, located at COPESUL - Companhia Petroquímica do Sul, are:

A) C6 Fractionator: it is part of the Benzene Production Unit, and its function is to separate, from a C5-C9 hydrocarbon mixture, one C6 cut in the top (rich in benzene), and a C7 + cut in the bottom.

B) Butene-1 Fractionator: it is function is to separate, from a C4 hydrocarbon mixture, butene-1 in the top with a minimal amount of n-butane.

C) Propylene Fractionator: it is function is to separate high purity propylene in the top (polymer grade, 99,50 %mol) from propane.

Table 1. Columns specifications

	A) C6 column	B) Butene-1 column	C) Propylene column
Column diameter, d_C (m)	1,85	2,54	4,40
Column height (m)	34,5	64,7	99,7
Number of trays	60	138	224
Feed tray	30	100	140
Tray type	Valve	dualflow	dualflow
Hole diameter, d_H (mm)	40	6	9
Trays spacing, T_S (m)	0,5	0,4	0,4
Light key	benzene	butene-1	propylene
Heavy key	toluene	n-butane	propane
Equation of state / Activity coef.	NRTL	SRK	RK-SOAVE
Binary interaction parameters	Dechema	Aspen *Ethylene*	Aspen Pure 12

3.2 Algorithm used

The Aspen Plus 12.1 simulator was used for carrying out the simulations. The implementation of the efficiency models, correlations for froth height over the tray, correlations for liquid entrainment and weeping, and mixture models of liquid over the tray were made with Fortran 77 programming language in the *calculator* block, and the algorithm used is showed in a summarized way in Figure 2.

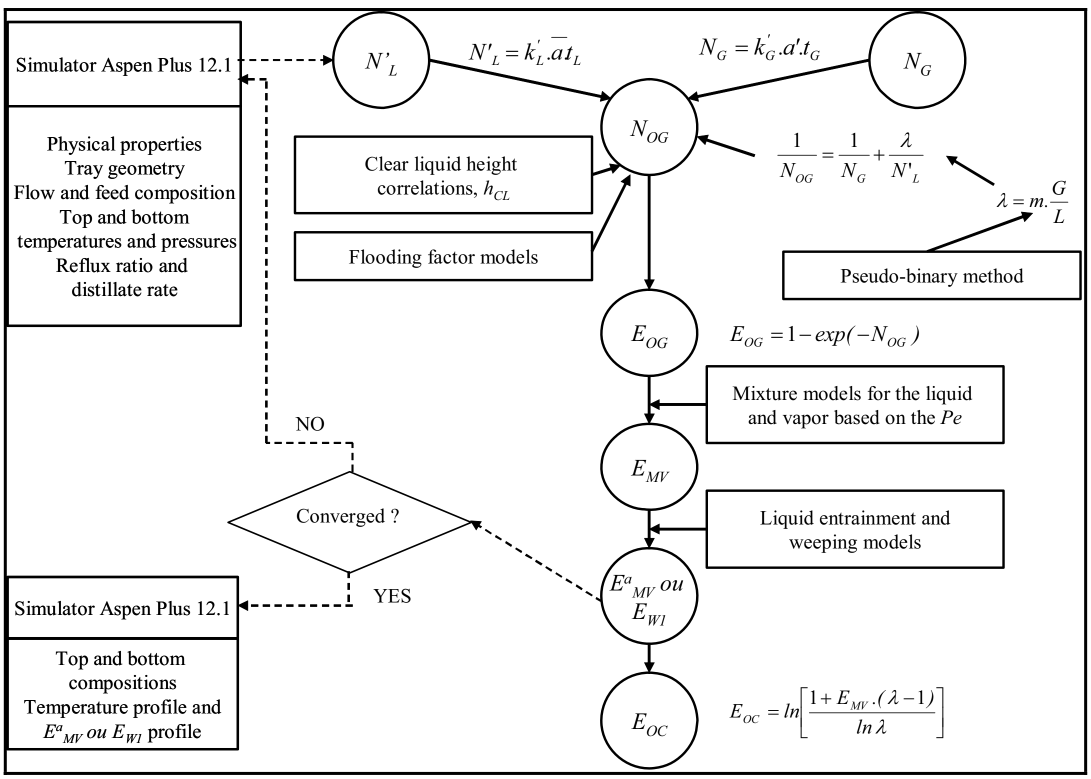

Fig. 2. Algorithm used in the Aspen Plus 12.1 simulator for the calculation of Murphree apparent tray efficiency (E^a_{MV} or E_{WI}).

4. Results and Discussion

The testing of the model by Garcia (1999) modified in the *FJ* parameter is shown in this Chapter. The validation of the suggested model is also presented, which will be referred as Garcia (1999) - modified, with the plant data. A comparison was also made with the Chan and Fair (1984) model for valve trays, and with the Xu et al. (1994) model for dualflow trays, as well as with the original Garcia (1999) model.

Figure 3, 4 and 5 shows, for several operational conditions, the overall efficiency values of the columns calculated by the efficiency prediction models, and compared with the overall efficiency values of the industrial columns.

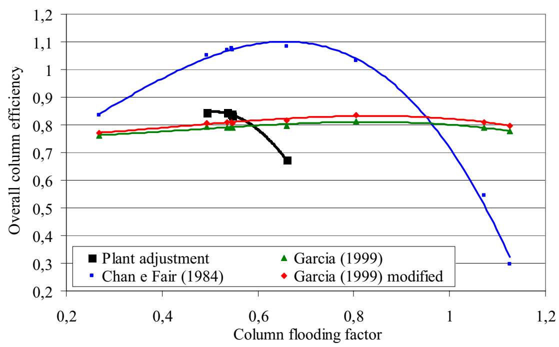

Fig. 3. Comparison of overall efficiency of the C6 column (valve tray) with the efficiency prediction models.

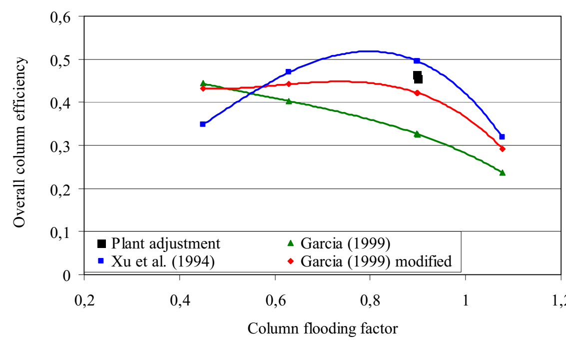

Fig. 4. Comparison of overall efficiency of the Propylene column (dualflow) with the efficiency prediction models.

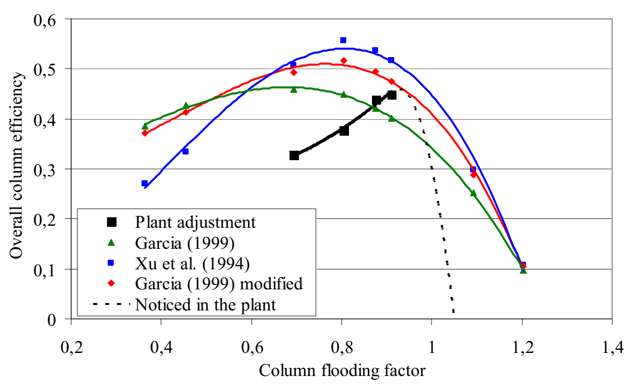

Fig. 5. Comparison of overall efficiency of the Butene-1 column (dualflow) with the efficiency prediction models.

The adjustment in the Garcia (1999) – modified model for the several actual column data was satisfactory. The $FJ_{modified}$ improved the overall efficiency estimate (E_{OC}) of the column for dualflow trays, in the case of the Propylene column. For the Butene-1 column results achieved are similar. In relation to the C6 column (valve trays) there was a slight improvement in the prediction of the column overall efficiency.

When a comparison is made between the original Garcia (1999) model and the modification suggested in this work, both have produced similar results, despite the fact that at the peak of efficiency, the modified Garcia

(1999) model was more accurate.

The models did not represented in a good way the sudden loss of efficiency above the 1,0 flooding factor. Above this value, there is a sudden loss in the column overall efficiency, as seen in the actual column (showed as the dotted lines in Figure 5).

Finally, the chart in Figure 6, show the compiled data from the three columns. Limits of ± 25 % are showed. These are reasonable limits for the adjustment of such diverse systems, geometries, operational conditions, analytical procedures, non-ideal thermodynamics degrees, and deviations in the material balance and other smaller deviations. One can observe that for the Garcia (1999) – modified model, from the 11 data points, only 1 is located out of limits. For Garcia (1999), without the modification in the *FJ* parameter, 3 points are out of limits. Finally, for the more used models by Chan e Fair (1984) for valve trays, and Xu et al. (1994) for dualflow trays, 3 points are out of the ± 25 % limits.

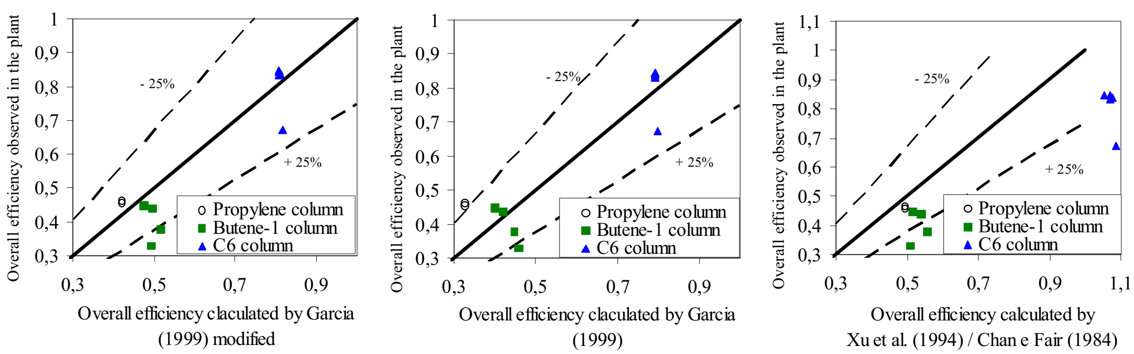

Fig. 6. Comparison between overall efficiency calculated by Garcia (1999) – modified, by Garcia (1999) original and by Chan e Fair (1984) and Xu et al. (1994), respectively values observed in industrial columns.

5. Conclusions

The Garcia (1999) – modified model for estimating the efficiency by contribution zones of mass transfer used in this work, coupled with the modifications suggested by Garcia e Fair (2002) specifically for dualflow trays, have successfully represented the dualflow tray performance (without downcomers and counter-current flow). This is one of the first attempts made for applying the Garcia (1999) / Garcia and Fair (2000) model in conjunction with the modifications suggested by Garcia and Fair (2002) in dualflow trays. The correction of the *FJ* parameter seemed coherent with the *jetting* fraction expected for such columns. Furthermore, this is also one of the first attempts of using the correlations suggested by Garcia and Fair (2002) for estimating the tray capacity (C_{SB}), liquid entrainment and weeping in dualflow trays.

The performance of Butene-1 and Propylene distillation columns were better represented by the modified model suggested in this work than by the previous models made by Garcia (1999) / Garcia and Fair (2000) and by Xu et al. (1994).

Another important aspect to mention is that, for dualflow trays, the Garcia (1999) modified model has represented the peak of efficiency closer to the plant reality than when using the original *FJ* suggested by Prado and Fair (1990) and originally used by Garcia (1999). The flooding factor range of 0,9 to 1,0, have the operation point where the columns work during almost 99 % of the time, and is also the most important operation range for the prediction of the overall column efficiency.

The use of the Garcia (1999) – modified model for the C6 column (valve tray) still deserves a certain reserve, since that it overestimate the *FJ* and the original Garcia (1999) model underestimate this factor. Both models were better than Chan and Fair (1984).

Another important contribution of this work was the implementation, in the Aspen Plus 12.1 simulator, of the algorithm for the calculation of the Murphree tray efficiency (E_{MV}) for use, in a quick manner, for the verification of efficiency in new tray distillation column designs in industry.

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Notation

A_A	Active or tray bubbling area ($A_T - 2.A_D$), m^2
A_H	Area of holes in tray deck, m^2
AJ	Fraction of small bubbles present in the bulk froth zone
a', $\bar{a}$	Interfacial area per unit volume of vapour and liquid, m^2/m^3
De	Eddy diffusivity for liquid mixing, m^2/s
d_J	Jet diameter, m
d_{BL}, d_{BS}	Arithmetic mean bubble diameter of large and small bubbles in the zones 2 e 4, m
d_{BLS}	Sauter mean bubble diameter of large bubbles in the zone 3, m

d_{BSS}	Sauter mean bubble diameter of small bubbles in the zone 5, m
d_C	Column diameter, m
d_H	Hole diameter, m
E_{OC}	Overall column efficiency
E_{OG}	Point efficiency
E_{MV}	Murphree vapour phase tray efficiency
E^a_{MV}	Apparent Murphree vapour phase tray efficiency, accounting the effects of entrainment and weeping of liquid in the valve trays
E_{W1}	Apparent Murphree vapour phase tray efficiency, accounting the effects of entrainment and weeping of liquid in the dualflow trays
FF	Flooding factor
FJ	Fraction of active holes that are jetting
FLB	Fraction of active holes that are issuing large bubbles
F_S	Superficial F factor = $u_A.\rho_G^{0,5}$, kg^{0,5}.m$^{-0,5}$.s^{-1}
FSB	Fraction of active holes that are issuing small bubbles
h_J	Jet height, m
h_{CL}	Clear liquid height, m
h_F	Froth height, m
h_W	Weir height or wave height in dualflow trays, m
k'_G , k'_L	Vapour and liquid phase mass transfer coefficient, m/s
L_W	Weir lenght, m
M_G, M_L	Mass vapour and liquid flow rate, kg/s
MW_G, MW_L	Molecular weight of vapour and liquid mixture, kg/kgmol
m	Slope of equilibrium line, dy / dx
N_G	Number of vapour phase transfer units: N_{G1} (Zone 1); N_{G2L} (Zone 2, large bubbles); N_{G2S} (Zone 2, small bubbles); N_{G3} (Zone 3); N_{G4L} (Zone 4, large bubbles); N_{G4S} (Zone 4, small bubbles); N_{G5} (Zone 5); N_{G6} (Zone 6); N_{GFJ} (Zones 1, 2 e 6); N_{GFLB} (Zones 3, 4 e 6); N_{GFSB} (Zones 5 e 6)
Q_G, Q_L	Volumetric vapour and liquid flow rate, m^3/s
Ts	Tray spacing, m
t_G	Mean residence time of gas in dispersion, s
u_A	Superficial gas velocity based on A_A or A_b, m/s
u_{AT}	Superficial gas velocity base on active área at the froth-to-spray transition point, m/s
$u_{A,0}$, $u_{A,100}$	Superficial gas velocity, base on active área at 0 % and 100 % jetting, m/s
Pe	Peclet dimensionless number: $Pe = \left(\frac{M_L}{MW_L}\right).d_C \Big/ L_W.h_{CL}.\left(\frac{\rho_L}{MW_L}\right).De$

Greek letters

ε,α	Vapour and liquid holdup fraction
λ	Ratio of slope of equilibrium line to slope of operating line: $\lambda = m.\left[\left(\frac{M_G}{MW_G}\right)\Big/\left(\frac{M_L}{MW_L}\right)\right]$
μ_G , μ_L	Vapour and liquid vicosity, Pa.s = kg/(m.s) = N.s/m^2
ρ_G, ρ_L	Vapour and liquid density, kg/m^3
σ	Surface tension, N/m
ϕ	Fraction perforated tray área (A_H/A_A)
η	Constant from Eq. 14: $\eta = \frac{Pe}{2}.\left[\sqrt{1+\frac{4.\lambda.E_{OG}}{Pe}}-1\right]$