

Assessment of separation efficiency modeling and visualization approaches pertaining to flow and mixing patterns on distillation trays

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1 **Review Article**

2 **ASSESSMENT OF SEPARATION EFFICIENCY MODELING AND VISUALI-**
3 **ZATION APPROACHES PERTAINING TO FLOW AND MIXING PATTERNS**
4 **ON DISTILLATION TRAYS**

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12
13 **Abstract:** Distillation columns are essential to chemical process industries, and most of them are
14 fitted with cross-flow trays due to their versatility. Since these columns are expensive in terms
15 of cost and energy consumption, an accurate determination of their separation efficiency is a
16 prerequisite to optimization of their performance by design modification and revamping. This
17 would further reduce the extra trays, added to account for the uncertainties, during the column
18 design leading to energy efficient operation. There have been several attempts in the past to
19 understand the nature of liquid mixing and flow patterns on the trays through experiments and
20 CFD simulations, and to relate them with their separation efficiency through CFD, empirical and
21 theoretical models. The present work aims at reviewing the experimental and the simulation
22 studies accomplished to characterize the flow and the mixing patterns on column trays. In par-
23 ticular, a comprehensive review of the existing theoretical efficiency prediction models along
24 with the critical analysis of their strengths and weaknesses is presented. The dependence of the

25 tray efficiency on system and flow properties is also discussed. In addition, a concise strategy on
26 how to process and utilize the experimental data in tandem with mathematical models is pro-
27 posed. The future of the tray efficiency modeling is anticipated to feature hybrid approaches, i.e.
28 using theoretical models supplemented with fluid dynamics information from experimentally
29 validated CFD models. Thus, the knowledge of the existing theoretical approaches is imperative
30 for their improvement and development of the new ones for better tray efficiency predictions.

31

32 **Keywords:** Distillation tray, tray efficiency, flow and mixing patterns, CFD, experiments, flow
33 maldistribution.

34

35 **1. Background**

36 Distillation is the most important separation technology and will be pursued in the future simply
37 due to the unavailability of industrially viable alternatives.¹ The physical separation of compo-
38 nent substances from their mixture, called feed, is achieved in distillation columns.² Distillation
39 columns are widely regarded as the workhorses of petroleum, chemical, petrochemical and re-
40 lated process industries.³ These units consume approximately 3% of the total energy of the
41 world,⁴ and about 50% of the total process energy in chemical and petroleum refineries.² They
42 also incur up to 50% of capital and operating costs in industrial processes.² These statistics cer-
43 tify distillation processes as the biggest energy consumers and the largest single investments in
44 chemical industries. Increasing energy costs and higher awareness for environmental concerns
45 motivate the scientific community to reconsider these cost- and energy-intensive process
46 equipments for improved designs as well as higher efficiencies.

47 Distillation columns are equipped with internals - primarily trays or packings or combination of
48 both.² The internals enhance the contact and the mass transfer between liquid and vapor phase
49 inside the column, which is essential for an efficient component separation. The selection of the

50 type of internals depends on several factors such as liquid and vapor load, operating pressure
51 and pressure drop, cost, sensitivity to fouling and corrosion, inspection access, revamping, expe-
52 rience and so forth.² Around half of the columns in the world are tray columns and the other half
53 are random and structured packing columns together.² The present work is concerned towards
54 the modeling approaches related with the columns fitted with cross-flow trays, which is the
55 most common tray configuration.² Further, as the column is a cascade of trays with more or less
56 same geometry and function, the modeling of the columns could be reduced to the consideration
57 of mass and enthalpy flow on one tray only.

58 The term 'efficiency' is preferred to account for the separation duty of a tray. However, several
59 definitions of efficiency, with reference to tray columns exist in the literature.⁵ The simplest in-
60 terpretation is the overall column efficiency (E_o), which is defined as

$$E_o = \frac{N_{eq}}{N_{ac}} \quad . \quad (1)$$

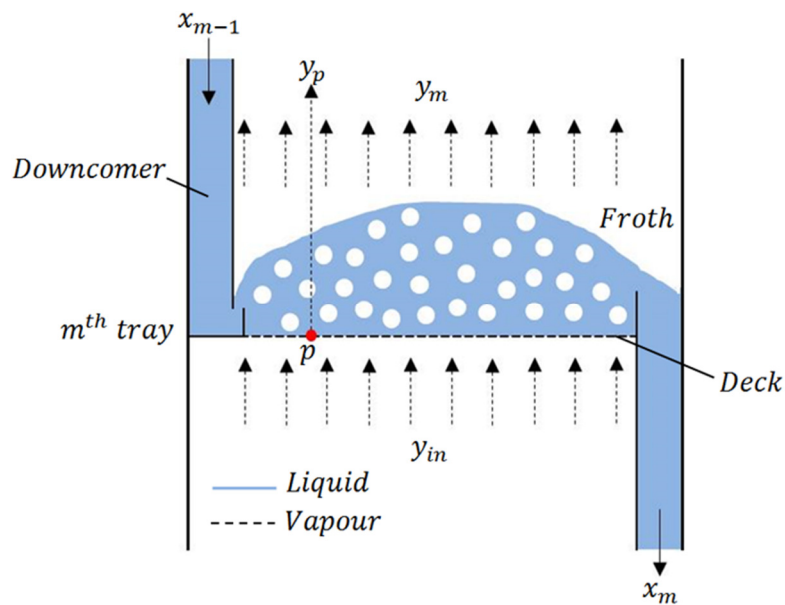
61 This is also known as the overall stage efficiency. Here, N_{eq} is the number of equilibrium stages,
62 obtained from equilibrium design calculations (McCabe-Thiele method), the Fenske-
63 Underwood-Gilliland method, process engineering softwares or from others,² while N_{ac} is the
64 actual number of trays in a column. The achievement of separation on a cross-flow tray is usual-
65 ly described by the (Murphree⁶) tray efficiency. It is the ratio of the actual change in vapor¹ com-
66 position on a tray over its composition change for an equivalent equilibrium stage, according to

$$E_{MV} = \frac{y_m - y_{in}}{y_m^* - y_{in}} \quad . \quad (2)$$

67 E_{MV} is the vapor-side tray efficiency as the composition change of vapor is considered. Here, y_m
68 is the composition of the vapor leaving the m^{th} tray whereas y_m^* is its composition in equilibri-
69 um with the liquid exiting the same tray (refer Fig. 1). The vapor composition y_{in} is homogenous
70 due to the assumption of perfectly mixed incoming vapor. This supposition has been practiced in

¹ The term 'gas' and 'vapor' are used interchangeably in this work.

71 numerous research articles and is only applicable to small diameter columns.⁷ Large columns
 72 often do not have sufficient distance between the consecutive trays for the vapor to get com-
 73 pletely mixed.⁷ Moreover, the Murphree tray efficiency is pertinent for completely mixed liquid,
 74 i.e. without any liquid concentration gradient on the tray, which does not happen in reality. For
 75 large columns and systems with high relative volatilities, the liquid composition x_m is some-
 76 times lower than its composition in equilibrium with the outgoing vapor i.e. y_m . Due to this rea-
 77 son, y_m^* becomes less than y_m , causing the tray efficiency to exceed unity.^{3,8}



78

79

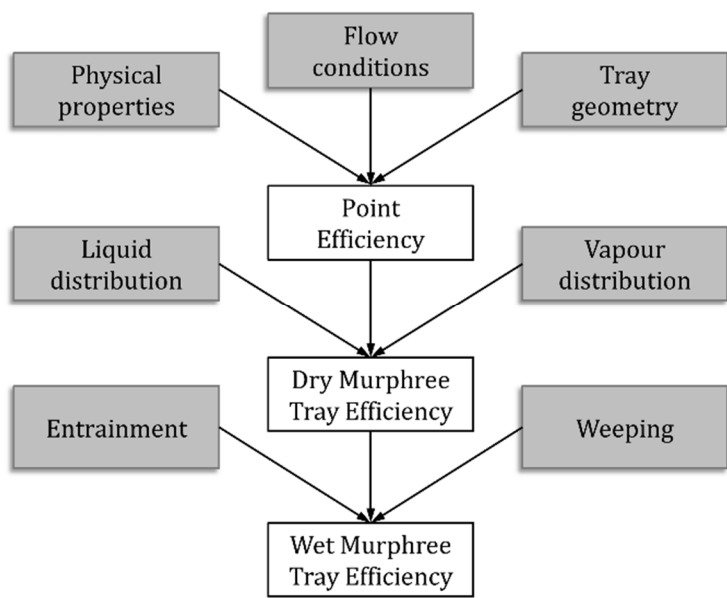
Fig. 1. Illustration for vapor-side tray and point efficiency.

80 Similar to the tray efficiency, the Murphree point efficiency is the actual composition change per
 81 equilibrium change at a particular point on the tray. The vapor-side point efficiency at point p on
 82 the tray is defined as

$$E_{OG} = \frac{y_p - y_{in}}{y_p^* - y_{in}} \quad (3)$$

83 y_p and y_p^* are the vapor compositions that are actual and in equilibrium with the liquid at that
 84 point, respectively, as shown in Fig. 1. This definition of the vapor-side point efficiency is more
 85 realistic than the tray efficiency as it considers the composition variation along the tray.² The
 86 difference between the vapor-side tray efficiency and the point efficiency arises due to the varia-

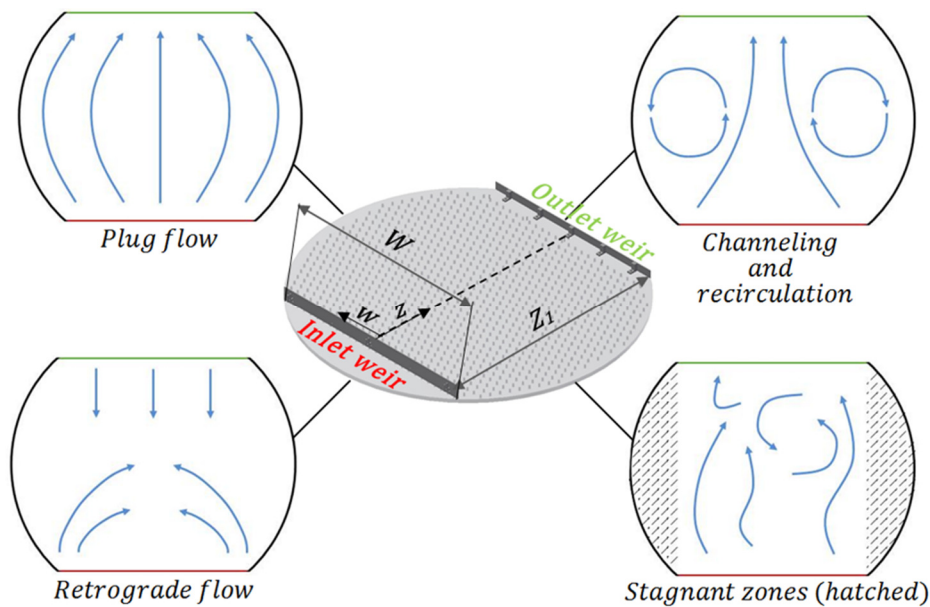
87 tion in the equilibrium vapor composition across the tray according to the liquid composition
 88 profile.⁹ Analogous expressions for liquid-side tray and point efficiency can be formulated.^{2,3} The
 89 tray efficiency is same as the point efficiency, when both liquid and vapor phases are completely
 90 mixed. However, the Murphree tray efficiency is usually higher than the point efficiency due to
 91 the cross-flow of gas and liquid.¹⁰ Other definitions of the tray efficiency were proposed for ex-
 92 ample by Hausen,¹¹ Standart,¹² and Holland^{13,14}. Recently, Jaćimović and Genić^{15,16} proposed the
 93 normalized tray efficiency (i.e. the ratio of the real tray mass transfer rate to the theoretical max-
 94 imum mass transfer rate), which is same for both phases and lies within zero and unity. The
 95 acknowledgement of any other efficiency concept than Murphree's by the process industry is yet
 96 to be noticed. Since the phases are partially mixed, a phenomenological model incorporating the
 97 mixing patterns of liquid and vapor is required for converting the point efficiency to the tray
 98 efficiency.³ Further, the efficiencies in Eqs. 3 and 4 are valid for binary mixtures. For multi-
 99 component mixtures, the pseudo-binary approach is preferred to retain the simple method with
 100 only minor changes.⁵



101
102 **Fig. 2.** Classification of the tray efficiency.

103 Further classification of the tray efficiency and the factors affecting it can be understood from
 104 Fig. 2.¹⁷ The point efficiency refers to the mass transfer at a certain point on the tray depending

105 on local flow conditions, physical properties of the fluids and geometry of the system. Similarly,
 106 the tray efficiency is a function of (i) geometrical design parameters of the tray, (ii) physical
 107 properties of the system (e.g. density, viscosity, surface tension, etc.) and (iii) overall operating
 108 conditions such as vapor and liquid loads. This efficiency is also known as 'Dry Murphree Tray
 109 Efficiency'. When the additional effects of entrainment and weeping (which are unfavorable for
 110 the tray or column performance) are further assimilated, the tray efficiency transforms to 'Wet
 111 Murphree efficiency'.¹⁷



112

113

Fig. 3. Liquid flow patterns on a tray.

114 The fashion in which the fluidic phases flow over the tray has strong influence on its mass trans-
 115 fer performance. Several studies concerning the experimental identification of the liquid flow at
 116 different design and operating conditions prompted the development of mathematical models to
 117 account for liquid maldistribution only. In general, the term 'flow non-idealities' is used to refer
 118 to liquid maldistribution. On the contrary, no attempts to quantify the vapor non-idealities
 119 through experiments have been made due to which the vapor flow is assumed in these models as
 120 stated earlier. Besides, the plug flow of liquid is known to be beneficial for the efficiency and is
 121 termed 'ideal' for the trays. On the other hand, non-ideal flow patterns, such as liquid channeling,

122 bypassing, retrograde flow and the presence of re-circulation and stagnant zones,¹⁸ as shown in
123 Fig. 3,¹⁹ are detrimental to the tray efficiency.²⁰

124

125 **2. Experimental and Numerical Flow Visualization**

126 Since the knowledge of the prevailing flow patterns is important for the evaluation of the tray
127 efficiency, different experimental and numerical techniques have been devised to visualize the
128 flow fields on the trays. These techniques are discussed successively hereafter.

129

130 **2.1 Experimental Studies**

131 The simplest experimental method involved the usage of floats, such as table-tennis or cork
132 balls, to pursue the flow of liquid.^{21,22} However, slip velocities between the liquid surface and the
133 balls as well as velocity gradients along the froth height limit the accuracy of this method. The
134 flow of liquid using colored dye and photographic camera was once visualized by Porter et al.²¹
135 In other studies, flow patterns were obtained from isotherms in the liquid, while the tray was
136 operated with hot water and cold air, and local liquid temperatures were measured with ther-
137 mocouples¹⁰ and thermometers²³ at multiple locations. Multiple flow pointers, like weather
138 vanes, were also used to detect the flow direction on a tray, despite of being highly intrusive to
139 the flow itself.²³ Yet, infrared camera technique was used to visualize the fronts of inflowing hot
140 liquid mixing with cold liquid.²⁴ The extraction of quantitative flow parameters with these tech-
141 niques was still difficult. The strain gauge probe technique was employed by Biddulph and Bulti-
142 tude²⁵ to obtain unidirectional velocity fields. However, the calibration of such probes is chal-
143 lenging, as they need to be adjusted for every froth condition. Solari and Bell²⁶ and Bell^{27,28} ex-
144 tensively utilized fiber optic techniques and fluorescent tracer to acquire flow and mixing pat-
145 terns using residence time profiles. Until now, the results from these experiments are preferably
146 used as validating criteria for numerical models (Computation Fluid Dynamics - CFD) discussed

147 later. Yu et al.²⁹ employed conductivity probes to trace the liquid flow using salt solution as trac-
148 er; however, the spatial resolution of recorded data is rather low. The nature of liquid flow at
149 different elevations above the tray deck was identified by Liu et al.³⁰ using a hot film anemome-
150 ter. Recently, Schubert et al.¹⁸ used a wire-mesh sensor to measure the residence time distribu-
151 tion and velocity fields distributed on a tray at uniquely high spatial and temporal resolution. A
152 consolidated list of existing experimental techniques to identify the flow behavior on column
153 trays is given in Tab. 1.

154

Space left for Table 1

Tab. 1. Summary of literature on experimental methods concerning column tray flow patterns.

Reference	Tray setup; gas/ liquid system	Technique	Observations
Stichlmair and Ulbrich¹⁰	$\emptyset = 2.30$ m bubble-cap and sieve tray; hot water/ air	Thermocouples	Liquid isotherms indicate the extent of channeling; influence of modified inlet and outlet weirs, tray tilting and baffles on flow patterns.
Biddulph and Bultitude²⁵	$\emptyset = 0.69$ m sieve tray; water/ air	Strain gauge probe network	Axial velocity profiles show non-uniform flow of liquid with low velocities near the wall.
Sohlo and Kinnunen²²	$\emptyset = 0.50$ m sieve tray; water/ air	Floating cork balls	Non-ideal velocity profiles at low liquid flow rates and at high weir heights; plug flow behavior at high liquid flow rates and at low weir heights.
Porter et al.²³	$\emptyset = 2.44$ m sieve tray; hot water/ air	Thermometers, flow pointers	Substantial liquid recirculation at high weir loads and at low gas loads.
Porter et al.²¹	$\emptyset = 1.20$ m sieve tray; water/ air	Photographic camera, dye injection, table-tennis balls	Existence of stagnant regions near the wall; tray tilting modifies the liquid flow patterns.
Solari and Bell²⁶	$\emptyset = 1.20$ m sieve tray; water/ air	Fiber-optic detection system, dye injection	Liquid pooling near the wall at low liquid and gas loads; effect of flow rates on this pooling; existence of non-ideal flow and mixing patterns.
Li et al.²⁴	$\emptyset = 1.20$ m sieve tray; water/ air	Thermal infrared camera, hot water injection	Flow non-uniformity on the tray with one downcomer; stagnant regions on multiple downcomer tray depicted through frontier curves.
Yu et al.²⁹	$\emptyset = 2.00$ m sieve tray; water/ air	Electrical conductivity probes, tracer injection	Non-uniform (parabolic) flow in the central part of the tray with slow recirculation near the wall.
Liu et al.³⁰	$\emptyset = 1.20$ m sieve tray; water/ air	Hot film anemometer	3D flow of liquid up to 10 mm above the tray deck and the flow becomes 2D beyond the aforementioned distance.
Schubert et al.¹⁸	$\emptyset = 0.80$ m sieve tray; water/ air	Wire mesh sensor, tracer injection	Influence of liquid load and outlet weir on flow patterns; liquid RTD and weir-to-weir velocities portraying flow non-idealities.

156 2.2 CFD Simulations

157 In addition to the advances in experimental techniques, CFD has progressively emerged as an
158 important tool³⁰⁻⁴² for understanding the complex two-phase flows on distillation trays and to
159 forecast the tray performance at best prior to construction for various designs and operating
160 conditions.³⁴ In the past 25 years, several attempts have been made to model the tray hydrody-
161 namics. All CFD studies discussed here use the Eulerian framework, if not otherwise specified.
162 Mehta et al.³¹ predicted the steady-state three-dimensional flow of the liquid on a sieve tray,
163 using time- and volume-averaged continuity and momentum equations for the liquid phase only.
164 Interactions with the vapor phase were considered using interphase momentum transfer coeffi-
165 cients determined from empirical correlations. Krishna et al.³² and Van Baten and Krishna³³ ad-
166 vanced the previous approach by proposing a three-dimensional two-phase model to simulate
167 the sieve tray hydrodynamics. They modeled the turbulent gas-liquid flow by assuming the mo-
168 mentum exchange through bubble-liquid interactions only. It should be further mentioned that
169 their work was focused on small trays, where fluid dynamics is inconsistent with that of indus-
170 trial trays. Also, they estimated the interphase momentum exchange coefficient based on the
171 correlation of Bennett et al.⁴³, which overpredicts the liquid holdup fraction in the froth regime.
172 Liu et al.³⁰ studied the two-phase flow behavior on a sieve tray with a relatively simple two-
173 dimensional model. They ignored the variations along the dispersion height in the direction of
174 gas flow, modeled the gas action with an empirical equation and described the hydrodynamics of
175 the liquid phase only. Gesit et al.³⁴ employed a three-dimensional model and used the liquid
176 holdup correlation suggested by Colwell⁴⁴ to predict the flow patterns and hydraulics of a com-
177 mercial-scale sieve tray. According to Kister³, different correlations can lead to inconsistent and
178 widely-varying predictions of the tray hydrodynamics.⁴⁵ Further, two-dimensional simulations
179 cannot account for the existing flow variations in the vertical dimension. Previously described
180 attempts were only concerned towards tray hydrodynamics, while they neglected mass and en-
181 ergy conservation on sieve trays. As a result, Wang et al.³⁵ established a three-dimensional pseu-
182 do-single-fluid model for obtaining liquid phase velocity and concentration distributions on

183 sieve trays in a 10-trayed column. A single-fluid model was preferred over a more accurate two-
184 phase model for simulating an entire column due to its simplicity and low computational cost.
185 They performed the mass transfer studies for cyclohexane – n-heptane system and estimated the
186 overall column efficiency using the Fenske-Underwood equation³⁵, which was overpredicted
187 with reference to Sakata and Yanagi⁴⁶. This method of determining the column efficiency using
188 end-product specifications is apt for approximate estimations only.⁴⁷ Error accumulation due to
189 simultaneous solution of momentum and mass-transfer equation and the usage of eddy-
190 diffusion coefficient from the correlations applicable for air-water system only are the other
191 reasons behind this overprediction. The assumption of constant values for vapor (and liquid)
192 volume fractions and the inability to predict point and tray efficiencies are further limitations of
193 this model. Rahimi et al.³⁶ and Noriler et al.^{37,38} extended the two-phase CFD model by consider-
194 ing the energy and the chemical species conservation in a three-dimensional framework. They
195 used correlations for momentum, heat and mass-transfer coefficients to predict hydrodynamics
196 along with temperature and concentration distributions on rectangular and circular sieve trays.
197 However, the employment of standard correlations and empirical models for simulating the heat
198 and mass-transfer on sieve trays is questionable.⁴⁷ Zarei et al.⁴⁸ compared the hydrodynamic
199 performance of a mini V-grid (MVG) valve tray and a sieve tray with a two-phase three-
200 dimensional model. The simulations indeed exhibited higher capacity for the MVG tray than for
201 the geometrically similar sieve tray, however, no experimental validation of the hydrodynamics
202 of MVG valve tray was attempted in their work. The effect of the holes and bubble diameters on
203 hydraulics and mass transfer performance of two geometrically similar sieve trays was investi-
204 gated by Rahimi et al.⁴⁹ using a three-dimensional two-phase model. They used a steady state
205 model, which is insufficient for modeling the dynamical behavior of distillation trays. Recently,
206 several investigators focused on the application of CFD studies to non-conventional trays. Jiang
207 et al.⁵⁰ and Li et al.³⁹ examined the tray hydraulics on a fixed valve tray through a two-phase
208 three-dimensional transient CFD model. Their models underpredicted the clear liquid height
209 with respect to experimental data. Jiang et al.⁵¹ developed a two-phase three-dimensional model

210 to study the hydrodynamics and mass-transfer behavior of a ripple tray, i.e. a special form of a
211 dual tray. A mismatch between CFD prediction and experiments concerning the froth height led
212 to a disagreement in the tray efficiency. Sun et al.⁵² used a three-dimensional two-phase model
213 with a realizable $k-\epsilon$ turbulence model to simulate the tray hydrodynamics on a cross-
214 orthogonal fixed valve tray. Similar analysis was also done by Li et al.⁴¹ for a sieve tray with flow-
215 guided holes and a bubble-promoter. The scope of their investigations were limited to hydrody-
216 namics, while their predictions were inconsistent with the correlations and experimental
217 data.^{41,52} Another study regarding the tray hydrodynamics in a sieve tray column under different
218 inclinations due to wind loads was conducted by Ping et al.⁴⁰ using the volume of fluid (VOF)
219 method. The interface curvature and surface tension forces are difficult to model correctly with
220 this model, thereby affecting the interface shape.⁵³ The prediction of clear liquid height through
221 this method was inconsistent with the Francis' equation and the experiment.⁴⁰ A hybrid ap-
222 proach of the volume of fluid (VOF) and a large eddy simulation (LES) model was developed by
223 Malvin et al.⁵⁴ to reduce the computational cost of the simulations. Although velocity predictions
224 were in good agreement with Solari and Bell²⁶ experiments, the same is not true for the clear
225 liquid height with respect to Solari and Bell²⁶, Colwell⁴⁴ and Bennett et al.⁴³. Li et al.⁵⁵ proposed
226 the concept of an 's' shaped distillation column fitted with elliptical sieve trays. They established
227 the importance of this unconventional tray by comparing its hydraulics, RTD and mass-transfer
228 performance with a conventional sieve tray, using two-phase three-dimensional model. Since no
229 such column exists in reality, this study lacked the experimental validation of the predictions.
230 Another unconventional tray known as conical cap (ConCap) tray was examined by Zarei et al.⁴²,
231 using a VOF-like code with multiple size group (MUSIG) and shear stress transport (SST) model.
232 The total pressure drop of the ConCap tray was underpredicted by their model with respect to
233 their experiments⁵⁶. A consolidated summary of the reported CFD analyses of distillation trays is
234 given in Tab. 2.

Tab. 2. Summary of literature on CFD studies for predicting the tray performance.

Reference	Multiphase model	Tray setup; gas / liquid system	Observations
Mehta et al. ³¹	3D, steady state, single phase, continuum based model	$\emptyset = 1.21$ m sieve tray; water/ air	Liquid velocity distribution
Krishna et al. ³²	3D, transient, two phase, Euler-Euler	0.39 m x 0.22 m sieve tray; water/ air	Liquid velocity vectors and streamlines, volume fraction distribution, liquid holdup distribution and clear liquid height
Van Baten and Krishna ³³		$\emptyset = 0.30$ m sieve tray; water/ air	
Liu et al. ³⁰	2D, steady state, single phase, $k-\epsilon$ turbulence model	$\emptyset = 1.20$ m sieve tray; water/ air	Liquid velocity vectors and circulation area
Gesit et al. ³⁴	3D, transient, two phase, Euler-Euler	$\emptyset = 1.22$ m sieve tray; water/ air	Velocity distribution and streamlines of liquid and gas, liquid velocity vectors, clear liquid height, froth height, liquid holdup and volume fraction profiles
Wang et al. ³⁵	3D, steady state, pseudo-single-phase, $k-\epsilon$ turbulence model	$\emptyset = 1.22$ m sieve trays (10 nos.) in a column; water/ air, and cyclohexane/ n-heptane	Liquid velocity distribution and vector plots, liquid concentration profiles and overall column efficiency
Rahimi et al. ³⁶	3D, transient, two phase, Euler-Euler	1.07 m x 0.09 m sieve tray; methanol/ n-propanol, and ethanol/ n-propanol. $\emptyset = 1.2$ m sieve tray; cyclohexane/ n-heptane	Liquid composition and temperature profiles, point and tray efficiency
Noriler et al. ^{37,38}	3D, transient, two phase, Euler-Euler	$\emptyset = 0.35$ m sieve tray; water/ air, and ethanol/ water	Liquid holdup, clear liquid height, pressure drop, gas and liquid velocity profiles and streamlines, liquid velocity and temperature distributions, mass and volume fraction, and point and tray efficiency
Zarei et al. ⁴⁸	3D, steady state, two phase, Euler-Euler	$\emptyset = 1.21$ m mini V-grid (MVG) valve and sieve tray; water/ air	Liquid velocity distribution, liquid and gas velocity vectors, clear liquid height, froth height, liquid holdup, pressure drop and liquid volume fraction profiles and streamlines
Jiang et al. ⁵⁰	3D, transient, two phase, Euler-Euler	$\emptyset = 0.60$ m fixed triangular valve tray; water/ air	Clear liquid height, holdup distribution and velocity vectors of gas and liquid, liquid velocity distribution and streamlines
Rahimi et al. ⁴⁹	3D, steady state, two phase, Euler-Euler	Two rectangular (0.99 m x 0.08m) sieve trays with different hole dia.; methanol/ n-propanol	Clear liquid height, froth height, liquid velocity profile, liquid and vapor phase mole fraction, liquid volume fraction contours, point and tray efficiency

Jiang et al. ⁵¹	3D, steady state, two phase, Euler–Euler	$\emptyset = 0.31$ m ripple trays with different free area; cyclohexane/ n-heptane	Clear liquid height, froth height, liquid velocity distribution and volume fraction, vapor phase mole fraction, interfacial area density and tray efficiency
Li et al. ³⁹	3D, transient, two phase, Euler–Euler	$\emptyset = 0.60$ m fixed valve tray; water/ air	Holdup distribution, velocity vectors and streamlines of liquid and gas, gas-liquid interface profile, clear liquid height and gas velocity distribution
Sun et al. ⁵²	3D, transient, two phase, Euler-Euler, realizable k - ϵ model	$\emptyset = 1.20$ m cross-orthogonal fixed-valve tray; water/ air	Clear liquid height, gas holdup profiles and liquid flow fields
Li et al. ⁴¹	3D, transient, two phase, Euler–Euler	$\emptyset = 0.57$ m sieve tray with flow-guided holes and bubble promoter; water/ air	Clear liquid height, liquid velocity distribution, liquid vector plots, streamlines and holdup distribution
Ping et al. ⁴⁰	3D, transient, two phase, VOF	$\emptyset = 0.38$ m sieve tray with 0-4° inclination; water/ air	Clear liquid height, liquid flow vectors and area of circulation
Malvin et al. ⁵⁴	3D, transient, VOF–LES	$\emptyset = 1.21$ m sieve tray; water/ air	Turbulent kinetic energy, clear liquid height, time-averaged liquid velocity profiles, droplet size distribution and mean sphere equivalent droplet diameter
Li et al. ⁵⁵	3D, steady state and steady–transient coupling, two phase, Euler-Euler	Elliptical (1.69 m x 0.85 m) and $\emptyset = 1.2$ m sieve trays; water/ air, and cyclohexane/ n-heptane	Clear liquid height, froth height, liquid and gas holdup distribution, liquid streamlines, liquid RTD, liquid phase molar fraction profiles and tray efficiency
Zarei et al. ⁴²	3D, transient, two phase, VOF-like method with MUSIG and SST model	$\emptyset = 1.20$ m conical cap (ConCap) tray; water/ air	Liquid volume fraction profiles, liquid and gas velocity vectors, total pressure drop and gas velocity variation along the height of cone

236 From the above model assessments, it can be easily observed that the majority of the hydrody-
237 namic simulations are conducted for air-water system only, and validated with the experiments
238 of Solari and Bell²⁶. Even though large columns can have very different flow patterns than ob-
239 served in the work of Solari and Bell²⁶. This is still considered as the state-of-the-art for CFD val-
240 idation irrespective of the recent experimental advances as mentioned in Tab 1. In addition, the
241 clear liquid height is considered as the sole criterion for the validation of the CFD studies. Veloci-
242 ty distribution and other hydraulic parameters should be used for this purpose to certify confi-
243 dence on the simulations. According to Schultes⁴⁵, the consideration of different correlations and
244 empirical equations (e.g. to model interphase momentum exchange and coefficients for heat and
245 mass transfer) leads to inconsistencies in the fluid dynamics, the separation efficiencies and the
246 specific mass transfer area. Further, CFD results should correlate with the experiments as close
247 as possible.⁴⁵ This is yet to be achieved for fluid dynamics due to which there is even more in-
248 consistency in the tray efficiencies from experiments and simulations, because of the dependen-
249 cy of CFD models on standard mass-transfer rate equations and empirical approaches for mass-
250 transfer coefficients.⁴⁷

251

252 **2.3 Objective Viewpoints**

253 Despite of the concerns regarding mass transfer predictions, it is clear that CFD will be the part
254 of the distillation modeler's toolbox in the near future to acquire the fluid dynamics on the trays.
255 Therefore, a hybrid strategy is expected in the future considering CFD simulations to obtain the
256 flow patterns and feeding them to mathematical models for efficiency predictions. The mathe-
257 matical models were developed, based on phenomenological relationships, to associate the flow
258 patterns and the liquid mixing with the tray efficiency. Since these models are an important pro-
259 spective to account the tray performance, it is crucial to discuss their formulation, which would
260 pave the way for their further evolution. To begin with the attributes of these models, some of
261 them do not take the account of non-ideal flow on tray efficiency despite of several attempts

262 regarding the measurement and simulations of flow non-uniformities. Instead, they simply as-
263 sume uniform liquid flow superimposed with mixing mechanism, uniform vapor flow with com-
264 plete mixing between the trays, linear equilibrium curve and so forth. As stated earlier, the uni-
265 form flow of homogenous vapor is only possible between small diameter trays.⁷ On large trays,
266 however, hydraulic gradients produce serious non-uniform vapor distributions.⁵⁷ Besides, few of
267 these models were formulated for rectangle-shaped trays.⁵⁸ The tray geometry, nevertheless,
268 plays a big role in shaping the flow on trays. The curved walls near the downcomer create the
269 tendency of directing liquid towards the tray centerline. This channeling causes the flow to sepa-
270 rate under certain conditions, thus, creating re-circulatory patterns.²⁸ In addition, Lockett and
271 Safekourdi²⁰ concluded that large deviations from the ideal velocity profile could be tolerated for
272 small to medium diameter trays without significant loss in efficiency as long as stagnant regions
273 are eliminated. The development of new or the modification of existing models to address and
274 verify these possibilities is inevitable. Therefore, it is highly important to revisit and compara-
275 tively analyze the formulation of the existing tray models with their strengths and weaknesses.
276 Recently, Taylor⁴⁷ also emphasized the need for understanding the formulation and solution of
277 the model equations.

278 The present work intends to congregate the existing efficiency prediction models so that their
279 characteristics can be discussed all-in-one place. A three-dimensional categorization of the
280 available models, based on tray resolution (in terms of mathematical segmentation), liquid mix-
281 ing and flow fields is presented in Fig. 4. Some models consider the whole tray while some seg-
282 ment the tray into channels and cells (pools) for material balancing. Flow patterns in terms of
283 velocities and stream functions are also incorporated in few models. The degree of liquid mixing
284 on a tray is specified on the third axis. An appropriate model should take incomplete liquid mix-
285 ing into account and hence, must lie between the extreme points of this axis. On the other hand,
286 an ideal model would be one that incorporates flow and mixing patterns at the best possible
287 resolution to predict the Murphree tray efficiency accurately. Furthermore, most of the models

302 and evaluates their effect on the tray separation performance. Further description about these
303 models is discussed henceforth.

304

305 **3.1 Basic Tray Models**

306 **3.1.1 Perfectly Mixed Model**

307 During the early 20th century, liquid on the tray was believed to be perfectly mixed due to the
308 agitating action of vapor rising through shallow pool of moving liquid. This assumption implies
309 the existence of a uniform liquid composition field. The vapor exiting the tray would also have
310 uniform composition for perfectly mixed vapor entering the tray. These viewpoints lead to

$$E_{MV} = E_{OG} \quad . \quad (4)$$

311 However, in 1934, Kirschbaum⁵⁹ observed gradients in the liquid composition on a small tray
312 (only few inches in diameter) at high superficial gas velocities. These findings led to the devel-
313 opment of tray models enlisted below.

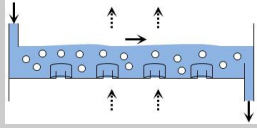
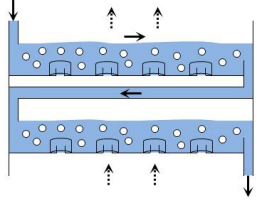
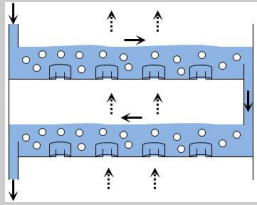
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315 **3.1.2 Plug Flow Model**

316 Lewis⁶⁰ firstly introduced the concept of plug flow on distillation trays. In this model, liquid is
317 assumed to travel across a rectangular bubble-cap tray without being mixed in the flow direc-
318 tion; however, there may be transverse mixing to any extent. The other assumptions are uniform
319 liquid and vapor loads, linear vapor-liquid equilibrium curve and constant point efficiency
320 throughout the tray. The material balancing over the tray yields the mathematical equations to
321 predict the tray efficiency given in Tab. 3 for three different cases according to the liquid flow
322 direction. These are the maximum achievable tray efficiencies for each case³. The efficiencies, in

323 actual, are lower due to the presence of mixing and non-uniformities in the liquid and the vapor
 324 flow.³

325 **Tab. 3.** Description of Lewis' plug flow model (→ liquid flow, ---→ vapor flow).

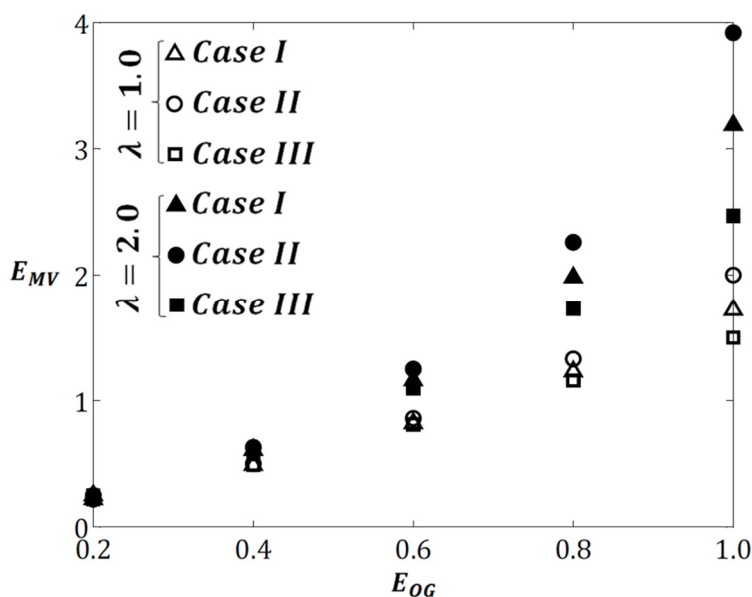
Cases	Description	Model
(I) Vapor entering the tray is completely mixed.		$E_{MV} = \{exp(\lambda E_{OG}) - 1\}/\lambda \quad (5)$ <p>λ is called stripping factor and is defined as</p> $\lambda = b \cdot G/L. \quad (6)$
(II) Unmixed vapor rises upwards, while liquid flows in the same direction on successive trays.		$E_{MV} = (\gamma - 1)/(\lambda - 1) \quad (7)$ $\lambda = \left(\frac{1}{E_{OG}} + \frac{1}{\gamma - 1}\right) \ln \gamma \quad (8)$
(III) All situations are identical to Case II except alternating flow of the liquid on successive trays.		$E_{MV} = (\gamma - 1)/(\lambda - 1) \quad (7)$ <p>For $\gamma < 1$:</p> $\lambda = \sqrt{\frac{\gamma^2 - (1 - E_{OG})^2}{E_{OG}^2(1 - \gamma^2)}} \cos^{-1} \left\{ 1 - \frac{(1 - \gamma)(\gamma - 1 + E_{OG})}{\gamma(2 - E_{OG})} \right\} \quad (9)$ <p>For $\gamma > 1$:</p> $\lambda = \sqrt{\frac{\gamma^2 - (1 - E_{OG})^2}{E_{OG}^2(\gamma^2 - 1)}} \cosh^{-1} \left\{ 1 + \frac{(\gamma - 1)(\gamma - 1 + E_{OG})}{\gamma(2 - E_{OG})} \right\} \quad (10)$

326

327 Fig. 5 illustrates the tray efficiency for each case graphically. Here, the efficiency is highest in
 328 Case II, followed by Case I and III, for the given values of λ . This is because the counter-current
 329 nature of contact between liquid and vapor phase is maximum during Case II, intermediate dur-
 330 ing Case I and minimum during Case III.³ However, since liquid flowing in the same direction on
 331 successive trays is uncommon,³ as shown in Case II, Case I is the most often used approach for
 332 efficiency predictions.³

333 The models discussed so far demonstrate the two extremes of liquid mixing on a tray. As already
 334 stated, it is impossible to achieve the efficiency predicted by them due to incomplete or partial

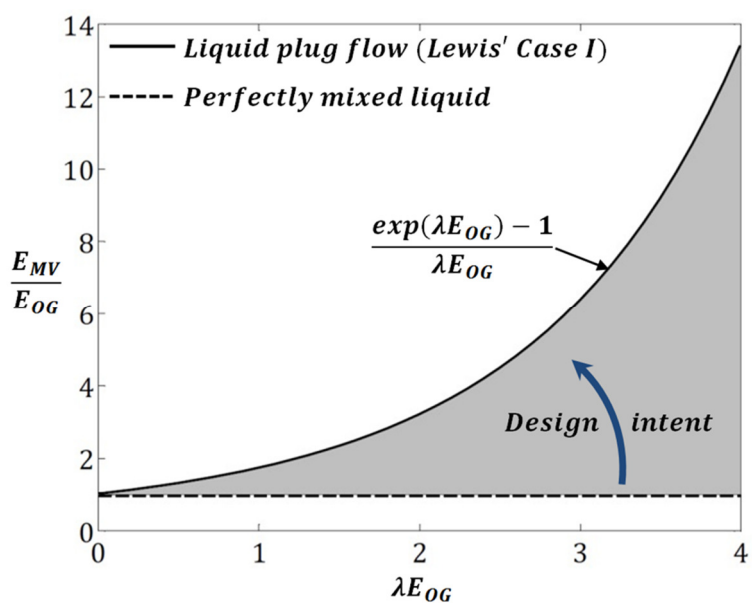
335 mixing of the liquid in reality. However, they provide an encapsulation of the separation efficien-
 336 cy, presented as a grey shaded area in Fig. 6, within which the efficiency of a tray with real flow
 337 and mixing conditions should always be.⁶¹ Strictly speaking, this holds only for the condition of
 338 completely mixed incoming vapor (i.e. uniform composition). Further, the intent of a distillation
 339 tray design should always be to approach the top (continuous) curve in Fig. 6, otherwise the tray
 340 would not fractionate as per expectations.



341

342

Fig. 5. Tray efficiency for the plug flow model.



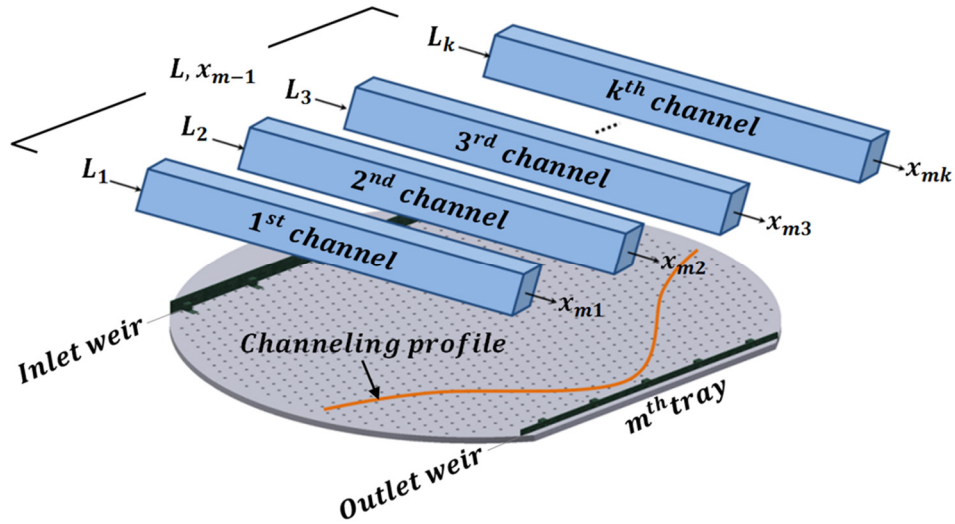
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344

Fig. 6. Tray efficiency for perfectly mixed liquid and plug flow.

345 **3.1.3 Multi-channel Plug Flow Model**

346 Stichlmair and Ulbrich¹⁰ observed channeling through distribution of liquid isotherms on bub-
 347 ble-cap and sieve trays. To account for liquid channeling in this model, the tray is assumed to
 348 consist of a large number of parallel channels, as depicted in Fig. 7. Plug flow behavior is as-
 349 sumed in each channel with different flow rates in accordance with the channeling profile. This
 350 assumption allows employing the Lewis' Case I to calculate the Murphree efficiency for each
 351 channel. This efficiency and the mass balance permit to find the liquid composition exiting each
 352 channel, for a given inlet composition. The averaging of the liquid composition from all channels
 353 enables to compute the tray efficiency.



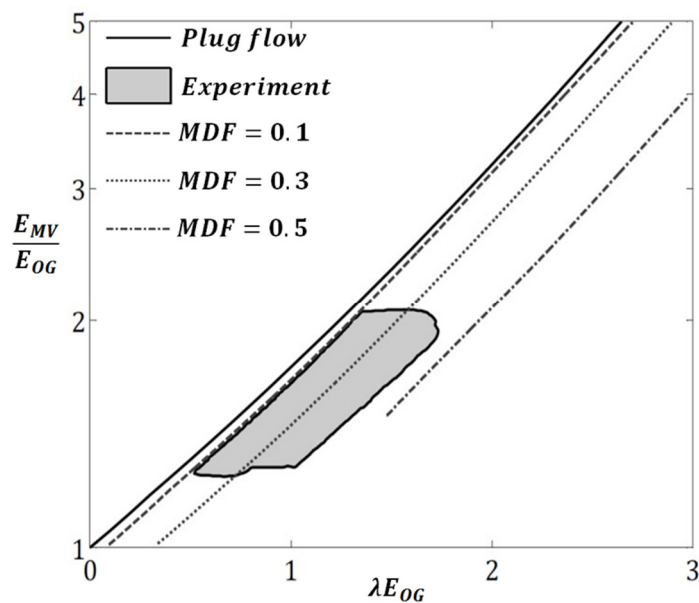
354
 355 **Fig. 7.** Stichlmair's multi-channel plug flow model.

356 The maldistribution factor, defined as

$$MDF = \frac{1}{L_{mean}} \sqrt{\frac{1}{k-1} \sum_{i=1}^k (L_i - L_{mean})^2} \quad , \quad (11)$$

357 was devised to correlate the consequence of channeling with the tray separation performance. It
 358 would be appropriate to call this factor as the coefficient of variation, as termed by Olujic' et al.⁶²
 359 for the packed columns. In fact, this factor represents the normalized variation of the local liquid
 360 flow and approaches zero for the plug flow situation. The efficiency according to the experi-

361 mental data, obtained by Stichlmair and Ulbrich¹⁰, is shown as the gray patch in Fig. 8. This fig-
 362 ure depicts the effect of channeling on the tray efficiency, from which it can be inferred that the
 363 tray performance suffers greatly in case of severe channeling. However, the straight relation
 364 between the MDF and the tray efficiency is not explained in the literature.¹⁰ Although this ap-
 365 proach allows capturing the effect of channeling, the application of this method for the non-
 366 idealities other than liquid channeling is disputable.



367
 368 **Fig. 8.** Effect of channeling on tray performance for multi-channel plug flow.

369
 370 **3.2 Liquid Pool Models**

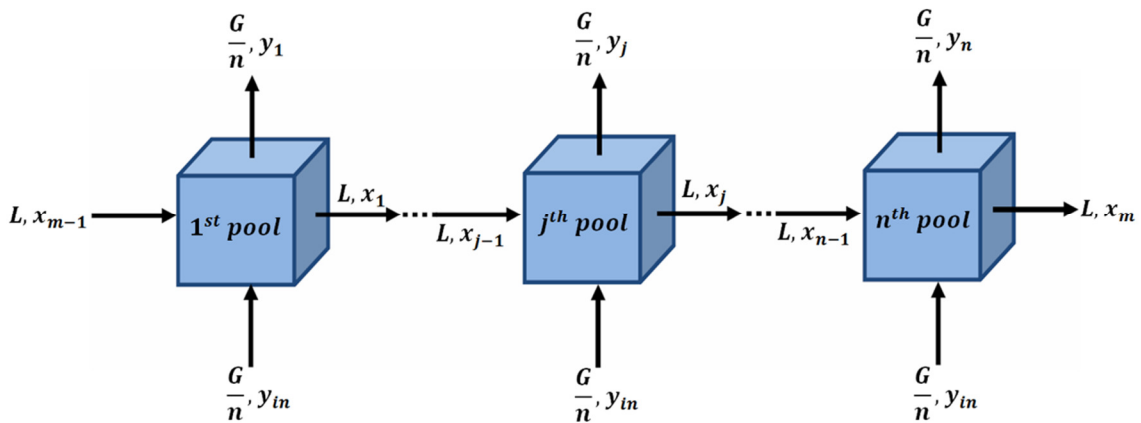
371 Kirschbaum⁶³ firstly proposed a model that considers the tray consisting of several identical
 372 pools of completely mixed liquid. These pools account for liquid concentration gradients in the
 373 flow direction. The liquid is assumed to flow through the pools one-by-one from inlet to outlet
 374 weir. A tray with one pool and with an infinite number of pools can easily explain the limiting
 375 cases of perfectly mixed and unmixed liquid, respectively. An intermediate number of pools cor-
 376 respond to incomplete or partial mixing of liquid.

378 **3.2.1 Mixed Stages Model**

379 Gautreaux and O’Connell⁶⁴ employed the Kirschbaum’s idea of perfectly mixed stages on separa-
 380 tion trays. They revisited the mixed pool concept and derived the equation

$$E_{MV} = \left[\left(1 + \frac{\lambda E_{OG}}{n} \right)^n - 1 \right] / \lambda \quad (12)$$

381 for n number of pools through material balancing on each stage (see Fig. 9), using the assump-
 382 tions similar to the Lewis’ case I except for liquid mixing. The derivation of the tray efficiency is
 383 simple and can be found in this publication.⁶⁴ The utility of this model was validated for the data
 384 obtained from a natural gasoline fractionator⁶⁵ (propane-butane system).⁶⁴



385
 386 **Fig. 9.** Schematic representation of the pool model with perfectly mixed liquid pools.

387 Fig. 10 presents the tray efficiency according to Eq. 12. A significant growth in efficiency with
 388 increase in n can be noticed. This observation holds for lower values of n , where the intensity of
 389 the efficiency rise is proportional to λE_{OG} . The tray efficiency reaches maximum with further
 390 increase in n and becomes stable thereby approaching the plug flow. This figure shows the tran-
 391 sition of the tray efficiency from the perfectly mixed liquid to the plug flow situation on the tray.
 392 For a fixed n , the gain in tray efficiency with increasing λE_{OG} is also evident. This observation is
 393 explained in Section 3.2.2.

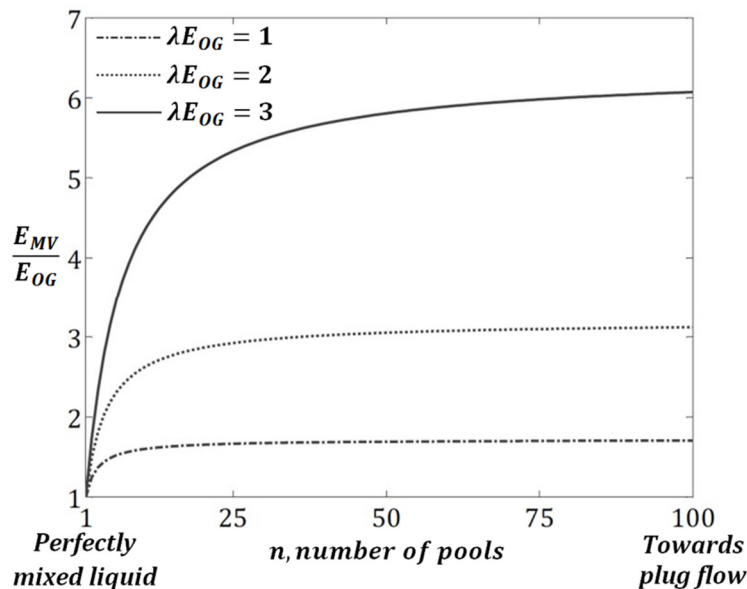
394 Initially, the determination of the number of pools equivalent to the actual liquid mixing in the
 395 flow direction was unclear. Miyauchi and Vermeulen⁶⁶ identified the mathematical analogy be-

396 between the axial dispersion model and the pool model assimilating backmixing amidst two con-
 397 secutive pools.⁶⁷ The parameters for quantifying the liquid mixing are Péclet number (Pe) and
 398 number of pools in the dispersion model and the pool model, respectively. Pe and n denote con-
 399 tinuous and discrete mixing in the respective methods. Further, Ashley and Haselden⁶⁸ con-
 400 firmed that the axial dispersion and the pool model are equivalent for

$$Pe = 2(n - 1), \text{ for } Pe > 2 \text{ and } \lambda E_{OG} < 0.5 \quad (13)$$

$$\text{and } Pe = 2n - 1 \text{ for large } Pe. \quad (14)$$

401 These observations were crucial for further developments in the pool modeling approach.

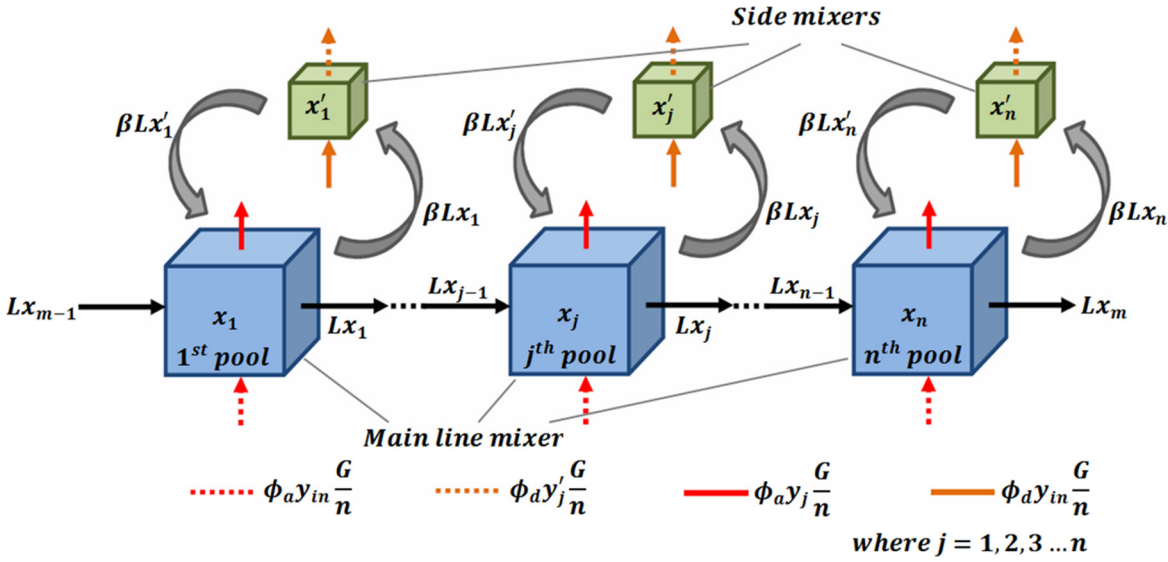


402
 403 **Fig. 10.** Tray efficiency versus number of stages for the pool model.

404 3.2.2 Pool Cascade Model

406 Bruin and Freije⁶⁷ formulated a simple and versatile ‘ready-to-use’ model to incorporate the
 407 effects of channeling and stagnant regions on the tray efficiency. Here, the term versatility refers
 408 to the applicability of this method to a single-pass cross-flow tray of any design. This approach
 409 assumes the tray to be comprised of a cascade of identical mixing cells called main line mixers.
 410 This is different to Kirschbaum’s concept, as each cell has a stagnant region in the form of a side

411 mixer connected to it. The main line mixers and the side mixers correspond to the active and the
 412 stagnant regions on the tray, respectively. According to Porter et al.²¹, the stagnant regions are
 413 that part of the froth or spray bed, where the flow is either stationary or circulating with closed
 414 streamlines, while those regions lying in the liquid flow path are termed as active regions.



415

416 **Fig. 11.** Schematic representation of the pool cascade model.

417 With reference to Fig. 11, the comprehensive detailing of liquid flow on the tray can be observed.
 418 This is a necessity to incorporate the active and stagnant regions in this model. Comparatively,
 419 the vapor flow is not similarly detailed as its average composition is considered here. The loss of
 420 information because of these simplifications is compensated by the introduction of parameters
 421 such as size of the active and the stagnant regions, and the exchange of liquid between main line
 422 and side mixers. Fig. 11 illustrates the working concept of this model. Liquid (L) flows through a
 423 cascade of main line mixers. A fraction of this liquid (β) is exchanged between the main line mix-
 424 er and its associated side mixer before passing on this liquid to the successive mixers. The in-
 425 formation on the relative volume of these mixers is reduced to their relative areas (ϕ_a and ϕ_d ,
 426 i.e. $\phi_a + \phi_d = 1$) due to the assumption of uniform froth height over the tray. The entry of the
 427 vapor proportional to the size of the corresponding mixer, constant point efficiency in each cell
 428 and linear VLE curve for an expected composition range are the other assumptions.

429 The mathematical modeling starts with the material balance in each cell. This enables to calcu-
 430 late the average vapor composition leaving the cells, which is compulsory to predict the tray
 431 efficiency. The material balance on j^{th} mixers provides the following equations

$$\text{Main line mixer: } L(x_j - x_{j-1}) + \beta L(x_j - x'_j) + \frac{G}{n} \phi_a (y_j - y_{in}) = 0 \quad (15)$$

$$\text{Side mixer: } \beta L(x_j - x'_j) + \frac{G}{n} \phi_d (y_{in} - y'_j) = 0 \quad (16)$$

432 The definition of the point efficiency provides important relationships for the j^{th} mixers as

$$\text{Main line mixer: } y_j = mE_{OG}x_j + (1 - E_{OG})y_{in} \quad (17)$$

$$\text{Side mixer: } y'_j = mE_{OG}x'_j + (1 - E_{OG})y_{in} \quad (18)$$

433 The average vapor composition exiting the tray can be obtained by using Eqs. 17 and 18 as

$$y_m = y_{in}(1 - E_{OG}) + mE_{OG}\phi_a \left\{ \sum_{j=1}^n \left(x_j + \frac{\phi_d}{\phi_a} x'_j \right) \right\} / n \quad (19)$$

434 By solving Eqs. 15 to 18 recursively followed by using Eq. 19 and the assumption of linear vapor-
 435 liquid equilibrium, the tray efficiency can be formulated as

$$E_{MV} = \left[\left[1 + \frac{\lambda E_{OG}}{n} \left\{ \phi_a + \phi_d / \left(1 + \frac{\lambda E_{OG} \phi_d}{n\beta} \right) \right\} \right]^n - 1 \right] / \lambda \quad (20)$$

436 Since λ , E_{OG} and n are usually known from system properties and mass transfer/residence time
 437 distribution correlations, ϕ_d (or ϕ_a) and β are the only adjustable parameters in the above equa-
 438 tion.⁶⁷ The tray efficiency in Eq. 20 accounts for liquid channeling and stagnant zones through
 439 these parameters. Further, the validity of Eq. 20 can be ensured by analyzing its transformation
 440 for the limiting cases of liquid mixing. For a tray with completely mixed liquid, i.e. with just one
 441 pool, β becomes infinitely large for a single cell due to which Eq. 20 transforms to Eq. 4. On the
 442 other hand, β is zero for plug flow, which changes Eq. 20 to

$$E_{MV} = \left[\left(1 + \frac{\phi_a \lambda E_{OG}}{n} \right)^n - 1 \right] / \lambda \quad . \quad (21)$$

443 An infinite number of cells correspond to liquid plug flow on a tray, which generates

$$E_{MV} = [exp(\phi_a \lambda E_{OG}) - 1] / \lambda \quad . \quad (22)$$

444 Appendix A describes the mathematical treatment on Eq. 21 to obtain the preceding equation.

445 This was reported by Porter et al.²¹ as the limiting solution for large trays without any liquid

446 mixing. As far as the calculation of number of pools (Eq. 13) is concerned, it is advised to prefer

447 the definition given by AIChE's bubble tray design manual⁶⁹ as

$$Pe = Z_1^2 / (D_E \cdot \tau) \quad . \quad (23)$$

448 This is the general definition of Pe , thus, it can be used for any tray design, and hence maintains

449 the model's versatility. Here, τ is the mean residence time of the liquid whereas D_E is the eddy

450 diffusion coefficient that defines the amount of liquid backmixing on the tray. This coefficient

451 depends on the flow characteristics and is influenced to a certain extent by the tray design.⁷⁰

452 Correlations for eddy diffusivity exist for a range of liquid and/or gas flow rates but are specific

453 to the tray design. An accurate determination of Pe or D_E is inevitable for unambiguous efficiency

454 calculations. The readers are referred to these publications^{22,29,71-79} for further information on

455 the degree of liquid mixing on trays.

456 Experiments and simulations regarding the flow visualization on trays are essential to this model

457 as they can provide the relative size of active and stagnant regions (i.e. ϕ_a and ϕ_d). To derive

458 β , the total exchanged flow between main line and side mixers is compared to the expected exchange

459 between active and stagnant regions by eddy diffusion.⁶⁷ Besides, the volatile material

460 transport to the rising vapor in a semi-infinite stagnant region is considered,⁶⁷ due to which the

461 steady state penetration depth of the volatile component from active towards stagnant region is

462 equivalent to the 'width of mixing zone'.²¹ This comparison and the subsequent simplifications

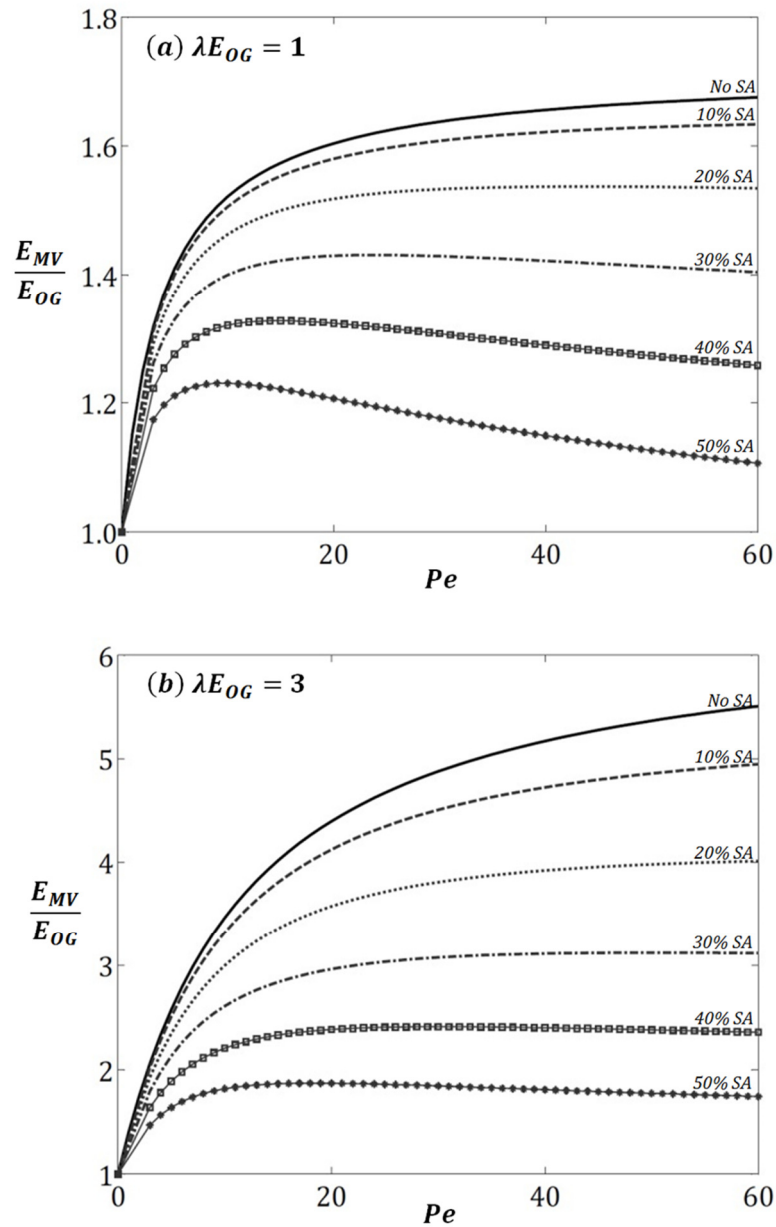
463 yield

$$\beta = \beta_o / \{ (1 + 0.5Pe) \sqrt{Pe} \} \quad . \quad (24)$$

464 The term β_o is an empirical fitting parameter and can be treated like a constant. This parameter
 465 can be calculated by using the above equation in conjunction with Eq. 20 for a system with
 466 known efficiencies. Bruin and Freije⁶⁷ recommended this parameter to be 4 as a first approxima-
 467 tion and validated the accuracy of this model through experimental data (Zuiderweg et al.⁸⁰ and
 468 Gerster et al.⁷⁴) and the eddy diffusion model²¹ (discussed in Section 3.3.2). The current model is
 469 in good agreement with the Porter's model²¹ but generally over-calculates the efficiencies by
 470 approximately 5-10% compared with the experimental data.

471 Considering the recommended value for β_o , Eq. 20 is illustrated graphically in Fig. 12 for the
 472 stagnant regions ranging from 10% to 50% of the tray perforated area. These results are pre-
 473 sented using Eqs. 13 and 24 for the λE_{OG} values as 1 and 3. The prediction of the tray efficiency
 474 in absence of any stagnant region (i.e. Eq. 12) is also shown here. It can be concluded that the
 475 size of the stagnant region is inversely proportional to the tray efficiency. The larger is the size of
 476 stagnant regions, the more serious is the loss in efficiency.²¹ For the given values of λE_{OG} , the
 477 efficiency loss is the highest for $\lambda E_{OG} = 3$. This inference is based upon the efficiency difference
 478 between no stagnant region and largest stagnant region curves for the corresponding values of
 479 Pe and λE_{OG} . Therefore, stagnant regions on the cross-flow trays should be eliminated as far as
 480 possible.

481 With reference to Eq. 23, the Péclet number is an indicator of the tray diameter as well as of the
 482 liquid mixing on the tray. Theoretically, high Péclet number corresponds to large-diameter trays
 483 as well as lower liquid mixing on them, and vice-versa.²¹ Liquid mixing in the flow direction (i.e.
 484 backmixing) is adverse to the tray efficiency, whereas transverse mixing is favourable for the
 485 tray performance.²⁰ Furthermore, λE_{OG} depends on the system and has an influence on the
 486 cross-flow mixing on a tray.²¹ Higher liquid mixing orthogonal to the flow direction can be ex-
 487 pected for an increase in λE_{OG} . All these information may help in better interpretation of the
 488 graphical results.



489

490

491 **Fig. 12.** Effect of channeling and dead zones on tray efficiency predicted by the pool cascade

492 model for (a) $\lambda E_{OG} = 1$ and (b) $\lambda E_{OG} = 3$.

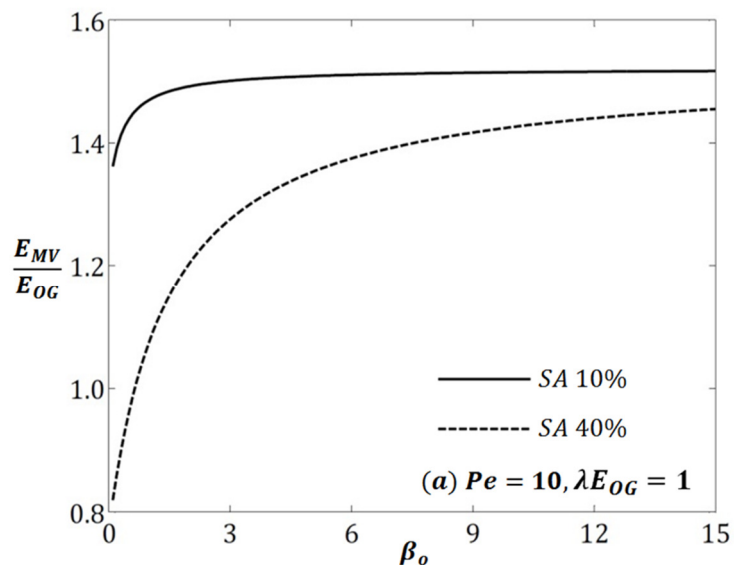
493 In Fig. 12, a sharp rise in the tray efficiency for low values of the Péclet number is visible. This
 494 means that transverse mixing of the liquid is dominant at this instant, which equalizes any flow
 495 non-uniformity on the tray.²⁰ In other words, the cross-flow liquid mixing on small trays is
 496 strong enough to wipe out the stagnant regions. This rise in efficiency with respect to the Péclet
 497 number becomes gradual and continues until the mixing in flow direction is less significant as
 498 compared to the transverse mixing. A further increase in the Péclet number refers to relatively
 499 larger trays, where the liquid cross-mixing is insufficient to deal with the flow non-idealities.

500 Due to this reason, large trays are susceptible to flow maldistribution and, therefore, no further
501 improvement in the tray performance happens thereafter. The location of this point, where no
502 improvement in the efficiency occurs, is dependent on the system and the flow parameters. The
503 situation becomes supportive for the formation of stagnant regions as the Péclet number further
504 increases. In addition to impeding the mass transfer, large dead zones can cause a significant
505 amount of vapor bypassing, too.²¹ These possibilities are evident in Fig. 12, where the tray effi-
506 ciency eventually drops for the stagnant regions larger than 20% of the tray bubbling area. Fur-
507 thermore, Porter et al.²¹ emphasized the tendency of λE_{OG} to oppose the vapor bypassing. Thus,
508 an increase in cross-flow mixing and higher resistance to vapor bypassing can be expected at
509 higher λE_{OG} . These are the reasons behind improvement in the tray efficiency with increase in
510 λE_{OG} . In addition, the position of the stagnant regions on large trays is also important. The ma-
511 jority of the mass transfer on such trays happens in their first half, near the inlet downcomer.⁵⁸
512 Therefore, the presence of any dead zone in the first half of a tray is highly disadvantageous for
513 their separation performance.

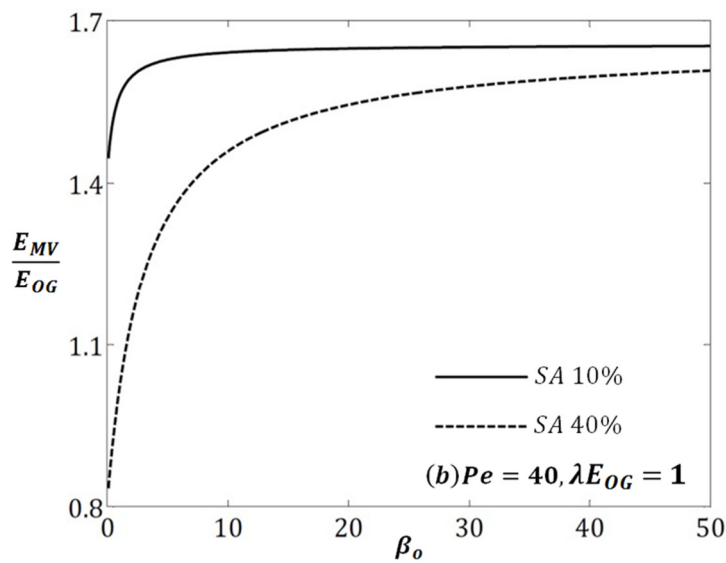
514 Fig. 13 aims at providing information on the selection of the empirical parameter β_o (Eq. 24) for
515 arbitrarily chosen values of Pe (10 and 40) and λE_{OG} (1). When Pe is 10, the maximum value of
516 β_o is 18.9, for which β is marginally less than unity. For Pe equal to 40, β is far less than unity
517 for the given range of β_o in Fig. 13b. The suggested value of this empirical parameter, i.e. 4 by
518 Bruin et al.⁶⁷, appear to be valid for small stagnant regions. This is because no significant change
519 is noticed in the efficiency after increasing this parameter. On the contrary, higher values of β_o
520 are suitable for the efficiency predictions, where stagnant areas are larger.

521 The conclusive remarks about this model is that it is simple, versatile, ready-to-use and, is able
522 to account for the effects of liquid channeling and stagnant regions on the tray efficiency. An
523 improvement in this approach could be achieved by incorporating the effect of other non-
524 uniformities in the liquid flow, such as retrograde flow and bypassing, as well as the location of
525 dead zones on the tray fractionation performance. The determination of active and stagnant

526 regions on a cross-flow tray, through simulations or experiments, has to be precise for this mod-
527 el to perform satisfactorily.



528



529

530 **Fig. 13.** Effect of the fitting parameter β_o on tray efficiency in the pool cascade model for (a)

531

$Pe = 10$ and (b) $Pe = 40$, at $\lambda E_{OG} = 1$.

532

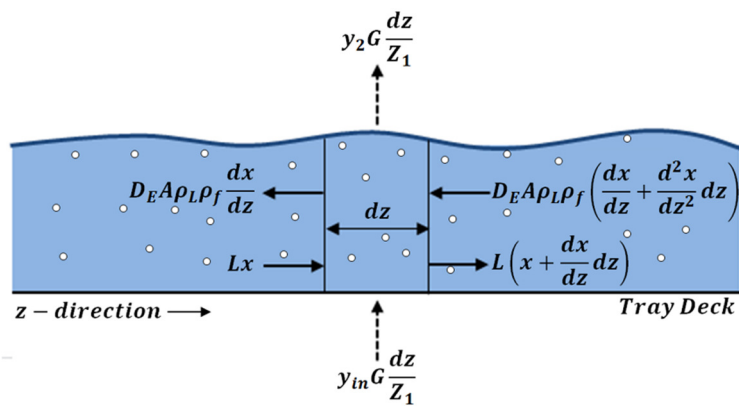
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534

535 **3.3 Diffusional Models**

536 **3.3.1 AIChE Model**

537 The AIChE model is the most widely applied and accepted model to predict the tray separation
 538 efficiency. In this approach, liquid is assumed to be mixed by the eddy diffusion mechanism, akin
 539 to molecular diffusion.⁷⁴ The rate of mass transfer from one tray location to another is assumed
 540 being proportional to the concentration gradient in the flow direction.⁷⁴ The proportionality
 541 factor is called eddy diffusion coefficient, which has already been described in the pool cascade
 542 model in Section 3.2.2. This mixing happens in conjunction with the mass transport by bulk flow
 543 of the liquid across a tray.⁷⁴



544

545

Fig. 14. Schematic representation of the AIChE model.

546 Although the concept of eddy diffusion is explained for a rectangular bubble-cap tray, it is ex-
 547 tendable to the trays of other design, too. Firstly, liquid and gas-phase transfer units are re-
 548 quired to find the point efficiency. Subsequently, they are used in a mathematical model to pre-
 549 dict the tray efficiency. Constant point efficiency and linear VLE curve are the assumptions in
 550 this model. Fig. 14 shows the liquid plug flow on the tray upon which the backmixing is super-
 551 imposed through eddy diffusion. The model starts with the mass balance on the vertical slice of
 552 the aerated liquid on the tray, which results in

$$D_E A \rho_L \rho_F \frac{d^2 x}{dz^2} - L \frac{dx}{dz} - G \frac{(y_2 - y_{in})}{Z_1} = 0 \quad . \quad (25)$$

553 Given the average froth velocity as $V_f = L/(A\rho_L\rho_F)$, normalizing the distance from the inlet weir
 554 in the flow direction as $s = z/Z_1$, and modifying the point efficiency as $E_{OG} =$
 555 $(y_2 - y_{in})/(y_2^* - y_{in}) = (y_2 - y_{in})/\{m(x - x_e^*)\}$, Eq. 25 transforms to

$$\frac{D_E}{V_f Z_1} \frac{d^2 x}{ds^2} - \frac{dx}{ds} - \lambda E_{OG}(x - x_e^*) = 0 \quad . \quad (26)$$

556 For convenience, the Péclet number in Eq. 23 is revised as $Pe = Z_1^2/(D_E \cdot \tau) = Z_1 \cdot (Z_1/\tau)/D_E =$
 557 $(Z_1 V_f)/D_E$. This simplifies Eq. 26 as

$$\frac{1}{Pe} \frac{d^2 x}{ds^2} - \frac{dx}{ds} - \lambda E_{OG}(x - x_e^*) = 0 \quad . \quad (27)$$

558 The boundary conditions for the above equation are

$$x|_{s=1} = x_m \quad \text{and} \quad (28)$$

$$\left. \frac{dx}{ds} \right|_{s=1} = 0 \quad .^{81} \quad (29)$$

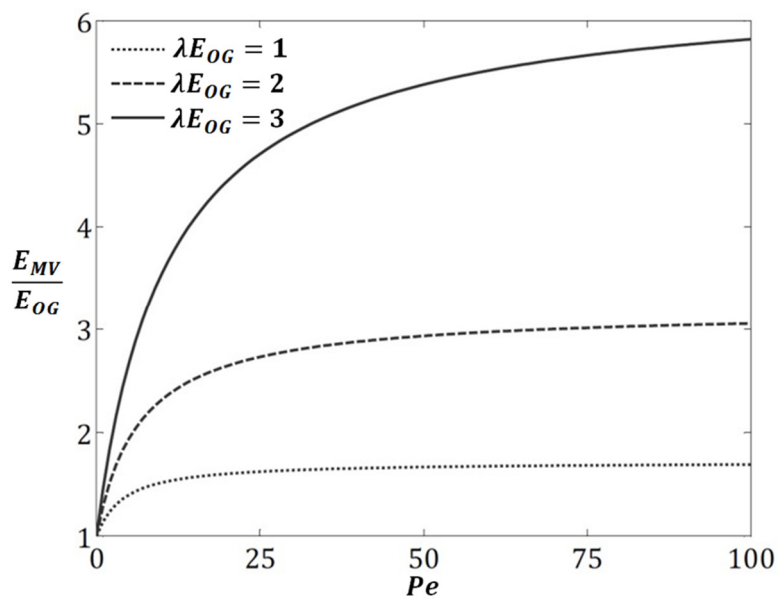
559 The second-order ordinary differential equation (Eq. 27) is solved in Appendix B for the given
 560 boundary conditions (Eqs. 28 and 29) and the final expression for the tray efficiency is

$$\frac{E_{MV}}{E_{OG}} = \frac{1 - \exp\{-(\eta + Pe)\}}{(\eta + Pe) \left(1 + \frac{\eta + Pe}{\eta}\right)} + \frac{\exp(\eta) - 1}{\eta \left(1 + \frac{\eta}{\eta + Pe}\right)} \quad (30)$$

$$\text{where } \eta = \frac{Pe}{2} \left(\sqrt{1 + \frac{4\lambda E_{OG}}{Pe}} - 1 \right) \quad . \quad (31)$$

561 Here, the tray efficiency depends on Pe and λE_{OG} only, out of which Pe requires an accurate de-
 562 termination of τ and D_E . As already mentioned in the pool cascade model, the eddy diffusion
 563 coefficient is influenced by the design of the tray.⁷⁰ The AIChE's report⁷⁴ gives a correlation of
 564 this coefficient for a rectangular bubble-cap tray; however, the flow patterns on circular trays
 565 can be very different than the idealized rectangular trays.²⁰ Further, the flow non-idealities are

566 the characteristics of circular trays, except those of very small diameter.⁵⁸ Therefore, it is ad-
 567 vised either to find the diffusion coefficient experimentally or to calculate it from correlations,
 568 for which the flow and the design parameters are within the range specified by the correlation.
 569 The efficiency predictions of this model have been validated for a 5.5 feet bubble-cap trayed col-
 570 umn (methyl dichloride – ethylene dichloride system).⁶⁹ The AIChE model agrees well with the
 571 experimental efficiencies when they are below 100%, however, the predictions are over-
 572 estimated, when the experimental efficiencies exceed unity.⁶⁹



573

574

Fig. 15. Tray efficiency prediction using the AIChE model.

575 Fig. 15 illustrates the impact of Péclet number and λE_{OG} on the tray efficiency. The significance
 576 of these non-dimensional parameters has been discussed in Section 3.2.2. A significant rise in
 577 efficiency with Péclet number is apparent for the low values of Péclet number. This is because
 578 the liquid mixing is significant on small trays, which eliminates the flow non-uniformities.²⁰ The
 579 intensity of this efficiency rise, as mentioned in the Section 3.2.1, is proportional to λE_{OG} . Such
 580 trend continues with increase in Péclet number until the liquid cross-mixing gets weaker and the
 581 bulk liquid velocity becomes dominant for the material transfer.²⁰ This causes the efficiency to
 582 rise with lower slope until it becomes constant.²⁰ The stagnation of tray efficiency is observable
 583 in Fig. 15 for all values of λE_{OG} except for $\lambda E_{OG} = 3$, where the efficiency becomes stable at very

584 high Pe , which is beyond the range of this figure. Since the cross-flow effect enhances with in-
585 creasing λE_{OG} , it is straightforward to expect a higher efficiency for higher values of Pe and
586 λE_{OG} . However, large trays are susceptible to flow non-idealities, stagnant regions and eventual-
587 ly vapor channeling due to which the efficiency should not rise but rather fall. Since this model is
588 designed to account for the liquid backmixing only, it is insensitive to non-uniform flow profiles
589 and stagnant regions. This could be the reason behind the efficiency overprediction by this mod-
590 el during its validation. Hence, Porter et al.²¹ named this model as ‘simple backmixing model’.
591 Further, several authors have further claimed that this model overestimates the tray
592 efficiency,^{21,58,67} which will be verified while comparing the results of the other models being
593 discussed. However, this model is still popular due to its simplicity and its ability to provide a
594 general estimate of the tray efficiency.

595

596 3.3.2 Eddy Diffusion Model

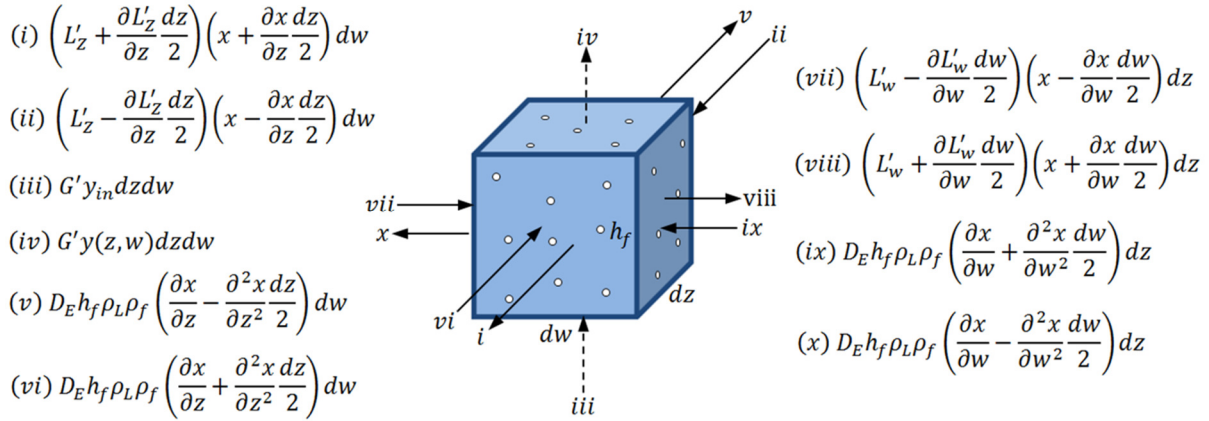
597 Porter et al.²¹ and Lim et al.⁸² developed the eddy diffusion model for single-pass and double-
598 pass cross-flow trays, respectively. These models account for liquid mixing in the flow direction
599 as well as in the transverse direction. Safekourdi⁵⁸ advanced these models by including liquid
600 velocities in terms of stream function over the bubbling area of the tray. The assumptions con-
601 sidered during the model formulation are

- 602 (i) constant point efficiency over the whole tray,
- 603 (ii) linear VLE curve for the expected composition range,
- 604 (iii) uniform liquid flow at the tray inlet,
- 605 (iv) completely mixed liquid and vapor entering the tray,
- 606 (v) perfect mixing of the liquid in the vertical direction in the froth, and
- 607 (vi) same eddy diffusivity in axial and transverse directions.

608 The coordinate system for a circular tray is shown in Fig. 3. Only half of the tray is considered
609 here due to symmetric concentration profiles on it.²⁶ An incremental area ($dz \cdot dw$) over the tray

610 having an aerated liquid (froth) with a uniform height h_f is considered. The transfer of mass into
 611 and out of this elemental froth is governed by the following mechanisms⁵⁸:

- 612 (i) mass transfer due to bulk movement of the liquid across the tray,
 613 (ii) mass transfer due to agitation of the liquid caused by the rising vapor, and
 614 (iii) mass transfer from liquid to vapor.



615
 616 **Fig. 16.** Mass balance over the froth element on m^{th} tray.

617 The mass balance over the froth element, depicted in Fig. 16, leads to

$$D_E h_f \rho_L \rho_f \left(\frac{\partial^2 x}{\partial z^2} + \frac{\partial^2 x}{\partial w^2} \right) - L'_z \frac{\partial x}{\partial z} - L'_w \frac{\partial x}{\partial w} - x \left(\frac{\partial L'_z}{\partial z} + \frac{\partial L'_w}{\partial w} \right) - G' \{ y(z, w) - y_{in} \} = 0 \quad (32)$$

618 Rearranging the above equation according to Appendix C gives

$$\frac{1}{Pe} \left(\frac{\partial^2 x}{\partial z'^2} + \frac{\partial^2 x}{\partial w'^2} \right) - \frac{W}{2D\psi_o} \left(\frac{\partial \psi}{\partial w'} \frac{\partial x}{\partial z'} - \frac{\partial \psi}{\partial z'} \frac{\partial x}{\partial w'} \right) - \frac{\lambda E_{OG} W D (x - x_e^*)}{A_b} = 0 \quad (33)$$

619 The boundary conditions for the liquid concentration and the stream function are

Centerline $\frac{\partial x}{\partial w'} = 0$ and $\psi = 0$ at $w' = 0$ and $0 \leq z' \leq \frac{Z_1}{D}$; (34)

Inlet $x_{+m} = x_{m-1} + \frac{1}{Pe} \frac{\partial x}{\partial z'}, \frac{\partial \psi}{\partial z'} = 0$ and $\frac{\partial \psi}{\partial w'} = \text{constant}$ at $z' = 0$ and $0 \leq w' \leq \frac{W}{2D}$; (35)

Wall $\frac{\partial x}{\partial n} = 0$ and $\psi = \psi_o$; at $0 \leq z' \leq \frac{Z_1}{D}$ and $\frac{W}{2D} \leq w' \leq \frac{1}{2}$; (36)

Outlet $\frac{\partial x}{\partial z'} = 0$ and ψ (shown graphically in Fig. 17); at $z' = \frac{Z_1}{D}$ and $0 \leq w' \leq \frac{W}{2D}$. (37)

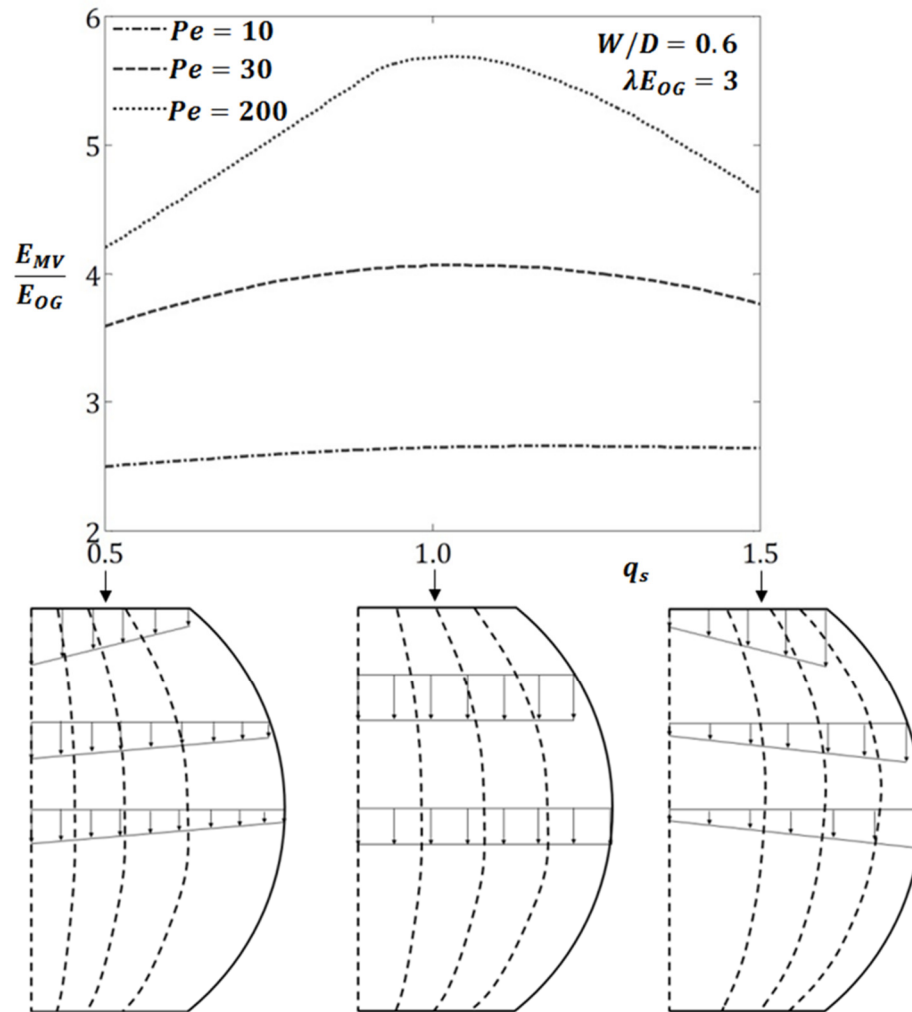
620 Eq. 33 is solved numerically with its associated boundary conditions using finite difference
 621 method. A detailed description on the finite-difference scheme, successive relaxation method
 622 and treatment of differentials near the wall are given in this publication.⁵⁸ Subsequently, the
 623 knowledge of the computed concentration profiles allows deriving the tray efficiency by follow-
 624 ing the treatment similar to Eqs. B8-B11 as

$$\frac{E_{MV}}{E_{OG}} = \left\{ \frac{1}{A_b} \int_{A_b} (x - x_e^*) dA_b \right\} / \left\{ \frac{1}{W} \int_{-W/2}^{W/2} (x_m - x_e^*) dw \right\} . \quad (38)$$

625 As per Eqs. 33 and 38, the tray efficiency is a function of liquid flow profile, Pe , tray design
 626 and λE_{OG} . The flow of liquid is assumed to vary linearly in the w -direction. The ratio of the liquid
 627 velocity at the wall and its mean value for any chord is denoted by q_s . Three values of q_s (0.5, 1.0
 628 and 1.5) are considered to account for three different velocity profiles, as shown in Fig. 17. The
 629 stream functions corresponding to each profile have been calculated and supplied to Eq. 33. All
 630 previously stated equations in this model were solved numerically and the efficiencies obtained
 631 for different values of Pe are shown in Fig. 17. It is straightforward that the efficiency is highest
 632 during the chordal flow of liquid ($q_s = 1.0$). In addition, a uniform residence time distribution
 633 exists on a tray at $Pe = 200$ and $q_s = 1$ due to which the efficiency approaches the solution of
 634 Lewis' plug flow model.⁶⁰ This does not happen for the profiles corresponding to q_s values of 0.5
 635 and 1.5.

636 As far as non-uniform flow patterns are concerned, the flow profile resembles the channeling
 637 for $q_s = 0.5$, i.e. having higher velocity at the tray centerline and lower velocity near the wall.
 638 This leads to stationary or decelerated regions close to the wall. Contrarily, no such possibility
 639 is anticipatable for $q_s = 1.5$ as near-the-wall velocities are larger than the centerline velocities.
 640 This could be a plausible explanation for higher efficiency in case of $q_s = 1.5$ than $q_s = 0.5$. Fur-
 641 ther, the computational ability and the validity of this model has been ensured by comparison

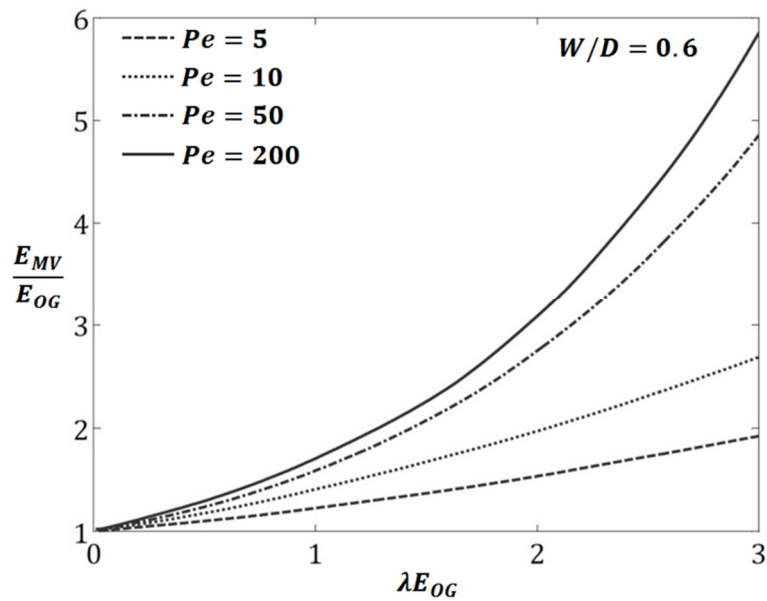
642 with the numerical solution of the AIChE⁶⁹ model. A slight overestimation of 3% in the efficiency
 643 required the predictions to be corrected by this value.⁸³ All results presented in this section have
 644 been corrected accordingly. The predictions from the model developed by Porter et al.²¹ was
 645 another criterion for the model authentication.



646
 647 **Fig. 17.** Tray efficiency for three different velocity profiles (dotted lines on the halved trays rep-
 648 resent the stream function for the corresponding velocity profile).

649 Fig. 18 shows the performance of the eddy diffusion model for the tray with uniform (optimal)
 650 liquid flow i.e. $q_s = 1.0$. The tray efficiency follows the same trend as in Fig. 15 due to similar
 651 reasons stated in Section 3.3.1. The calculation of the concentration profiles on a tray corre-
 652 sponding to the liquid flow profile and subsequent determination of the tray efficiency demands

653 plenty of computational effort. On the other hand, this remains the only model that considers
 654 liquid dispersion in the traverse as well as in the flow direction.

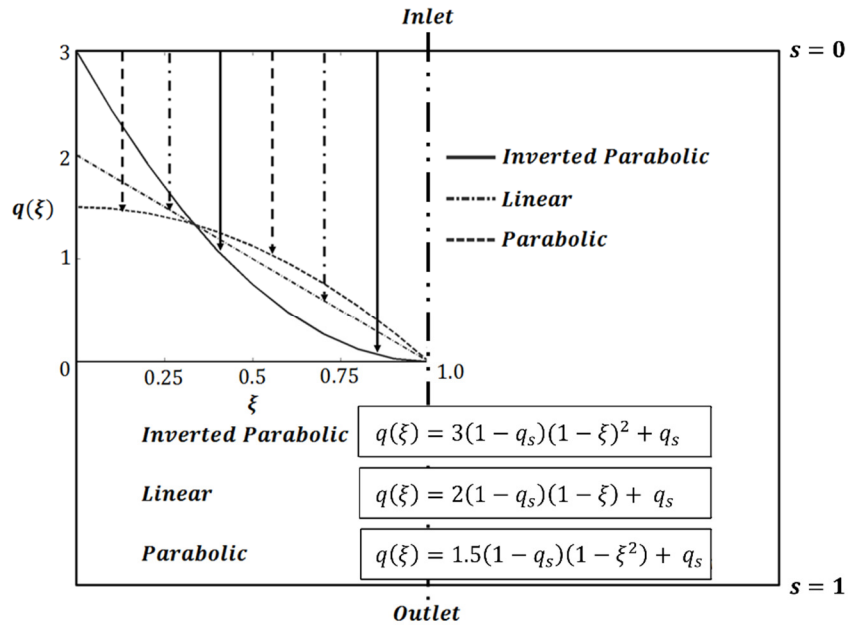


655
 656 **Fig. 18.** Tray efficiency prediction for the optimum velocity profile by the eddy diffusion model.

657

658 3.4 Non-uniform Flow Model

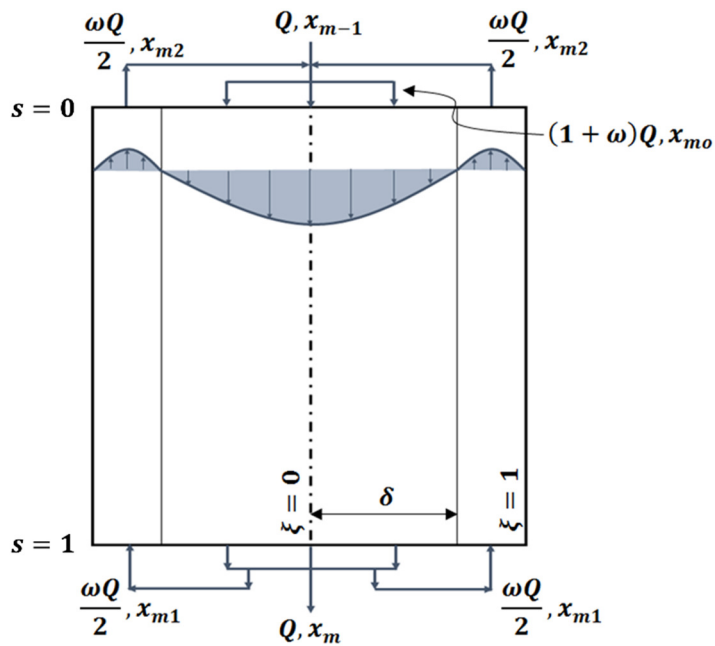
659 The current model analyzes the effect of non-uniform velocity distributions, in the absence of
 660 liquid mixing, on the tray efficiency.⁸⁴ The absence of liquid mixing is essential to sustain a veloc-
 661 ity profile throughout the tray. Although this concept is purely theoretical, it allows distinguish-
 662 ing between the effects of various flow patterns on the tray performance. The model considers
 663 two variations⁸⁴: one for simple non-uniform velocities and the other for retrograde flow along-
 664 side non-uniform velocity distributions. For simplicity, a rectangular tray was assumed to derive
 665 the mathematical model. However, the model could be easily extended to circular tray geome-
 666 tries by increasing the flow path length near the wall.⁸⁴ No concentration gradients in the direc-
 667 tion normal to the main flow have been assumed. The coordinate system of this model is given in
 668 Fig. 19a.



669

670

(a)



671

672

(b)

673

Fig. 19. (a) Co-ordinate system with velocity distributions for the simple non-uniform flow

674

model for $q_s = 0$ and (b) schematics of the retrograde flow model.

675

Bell²⁸ and Solari⁸³ reported the general mass transport equation for a binary system, derived

676

from the species continuity equation, as

$$q \cdot \nabla x - \nabla \cdot (Pe^{-1}) \cdot \nabla x - \lambda E_{OG} \{x_e^* - x(s, \xi)\} = 0 \quad . \quad (39)$$

677 This steady-state equation forms the basis of this model. The vector q is an arbitrary velocity
678 field that is normalized by the average velocity corresponding to the uniform flow on the same
679 tray and at the same flow rate. Uniform inlet vapor composition, linear VLE curve and constant
680 λE_{OG} are the assumptions applied here. In addition, Pe is the Péclet number denoting the three-
681 dimensional eddy mixing. It is taken as infinity due to the assumption of no mixing on the tray.
682 This simplifies the above equation as

$$\frac{dx(s, \xi)}{ds} - \frac{\lambda E_{OG}}{q(\xi)} \{x_e^* - x(s, \xi)\} = 0 \quad . \quad (40)$$

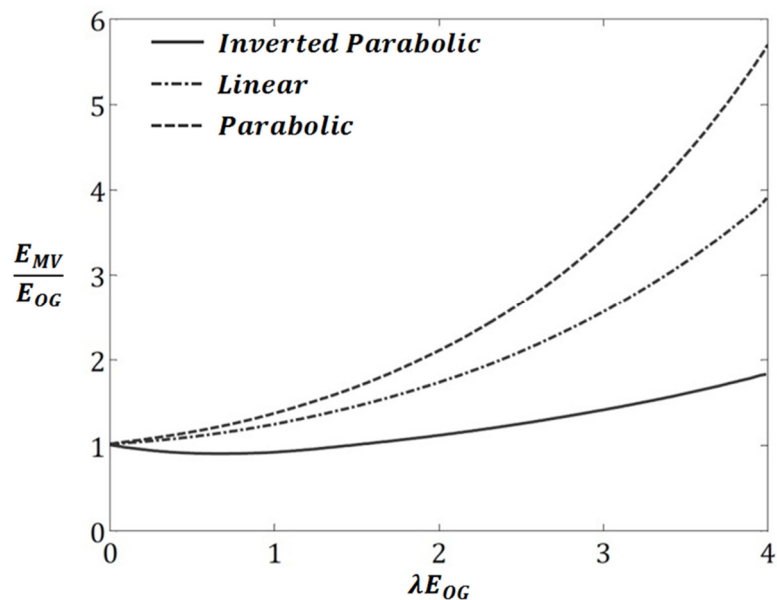
683 Eq. 40 is solved for $x(s, \xi)$ by the method of separation of variables and subsequently used in the
684 definitions of tray and point efficiency, which leads to

$$\frac{E_{MV}}{E_{OG}} = \frac{\left[\int_0^1 \frac{q(\xi)}{\lambda E_{OG}} \left\{ 1 - \exp\left(-\frac{\lambda E_{OG}}{q(\xi)}\right) \right\} d\xi \right]}{\left[\int_0^1 q(\xi) \left\{ \exp\left(-\frac{\lambda E_{OG}}{q(\xi)}\right) \right\} d\xi \right]} \quad . \quad (41)$$

685 Three velocity distributions, namely inverted parabolic, linear and parabolic (see Fig. 19a) are
686 analyzed here. The inverted parabolic distribution corresponds to severe channeling along the
687 tray centerline, while the parabolic distribution closely resembles the uniform flow. q_s is the
688 normalized slip velocity at the wall and is considered zero in Fig. 19a for simplicity. It is also a
689 measure of intensity of the non-uniformity as shown by the equations mentioned in Fig. 19a.

690 Fig. 20 reveals the impact of these velocity distributions on the tray separation performance.
691 Due to resemblance with uniform flow, the parabolic distribution seems more advantageous for
692 the tray functioning than its counterparts. The efficiency-alleviating effect is the highest for the
693 inverted parabolic distribution as it replicates severe liquid channeling on the tray. The efficien-
694 cy of the linear distribution is intermediate between the other two profiles, as its flow intensity
695 also lies amidst the other two distributions. This figure also confirms that a significant im-
696 provement in the tray efficiency with increase in λE_{OG} is only possible for uniform liquid flow,
697 i.e. parabolic velocity distribution. Hence, the difference in the separation performance of these
698 distributions is larger at higher values of λE_{OG} .

699 A peculiar observation about the inverted parabolic profile is that the E_{MV}/E_{OG} ratio at smaller
700 values of λE_{OG} is less than unity for this distribution with a zero slip velocity at the wall. Foss et
701 al.⁷³ also proclaimed the drop of the tray efficiency below point efficiency that approaches zero
702 for bypassing liquid. This fact contradicts the possibility of the tray efficiency to fall between the
703 mixing extremes on a tray, as shown in Fig. 6. However, in reality, this observation can be ques-
704 tioned as no such occurrence is reported in the AIChE analysis.⁷⁴ Besides, this model is one of the
705 standalone methods that consider a liquid velocity profile at the tray inlet other than plug flow,
706 as it can easily distinguish between the effects of these profiles on the tray performance.



707
708 **Fig. 20.** Effect of different velocity profiles on tray efficiency from the non-uniform flow model.

709 Similar to the simple non-uniform flow model, Bell and Solari⁸⁴ devised another model by ac-
710 commodating a retrograde flow on either side of the forward flow path, as demonstrated in Fig.
711 19b. The forward and the retrograde flow regions are separated by a line, where the liquid ve-
712 locity is zero. This type of model has been termed as the ‘non-uniform retrograde flow model’
713 and is further classified into two sub-categories. In the first model, the liquid flowing through the
714 forward flow path is perfectly mixed at the outlet. A fraction of this uniform composition liquid
715 is diverted to the retrograde flow path and is called as ‘uniform composition model’ (as shown in
716 Fig. 19b). In the second model (not shown here), some of the flow paths of the liquid near zero

717 velocity line are directly rotated to the retrograde flow region and is therefore named as 'exter-
718 nal rotation model'. This causes the liquid near the tray centerline in the forward flow region to
719 flow near the wall in the retrograde flow region. Here, the liquid composition varies across the
720 inlet of the retrograde zone opposite to the uniform composition model. The expression of the
721 tray efficiency for these cases can be derived by following a similar procedure as employed in
722 the simple non-uniform flow model.⁸⁴

723

724 **3.5 Residence Time Distribution (RTD) Model**

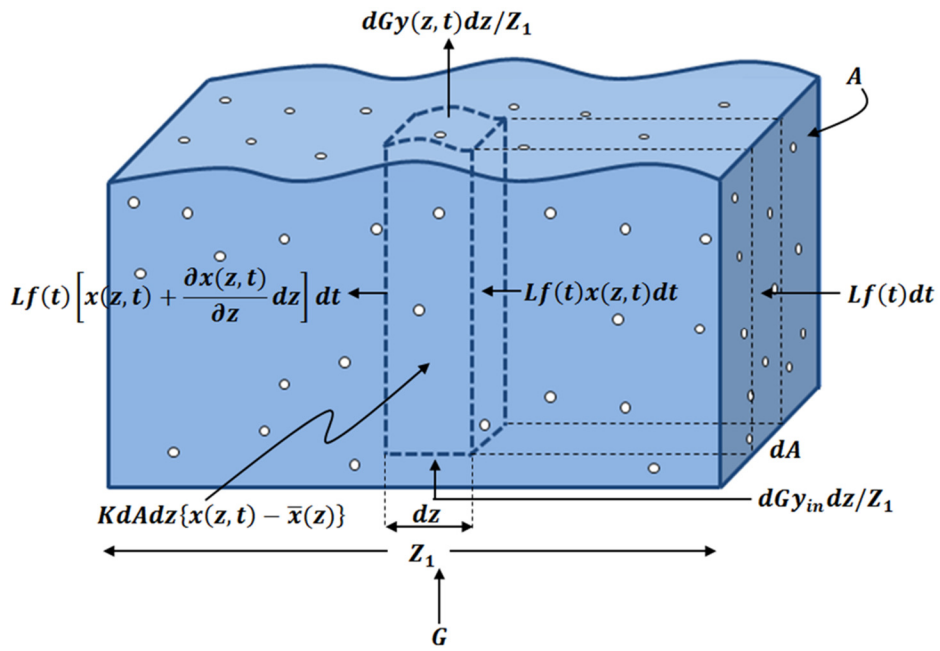
725 The RTD model employs the residence time concept to characterize the degree of liquid mixing
726 on a tray. This method assumes that the mixing of liquid produces a distribution of residence
727 time, ranging from zero to infinity.^{73,85} This approach is capable of establishing the nature and
728 the extent of all possible types of liquid mixing on various trays, indicating the superiority of this
729 method over the existing models.

730 The concept of residence time is well-known and has been subjected to numerous studies in
731 interdisciplinary fields.⁸⁶⁻⁸⁸ Danckwerts⁸⁹ presented the unified and comprehensive treatment of
732 this concept in continuous flow systems, after which the RTD studies gained large recognition
733 and found application in chemical and reaction engineering. The experimental determination of
734 the RTD based upon injection and dispersion of appropriate tracers, known as stimulus-
735 response method, is discussed in detail in the literature.⁹⁰

736 Fig. 21 shows the cross-flow of the liquid on the tray. The following assumptions are considered
737 to formulate this model:

- 738 (i) liquid entering the tray consists of an infinite number of streams, each of which resides
739 for a certain time on the tray,
- 740 (ii) plug flow of uniform gas through the liquid above the tray,
- 741 (iii) complete mixing of liquid in the vertical direction, and

742 (iv) linear VLE curve.



743

744

Fig. 21. Schematic representation of the RTD model.

745 The concentration of the dissolved material in each stream is affected by the mass transfer to the
 746 gas at local efficiency and by exchange with its local surroundings.⁸⁵ A froth element residing on
 747 the tray for a time ranging between t and $t + dt$ is subjected to the mass balancing. The total
 748 material balance over the whole tray can be setup by summation over all fluid elements, if their
 749 residence time distribution is known. Fig. 21 displays an aerated element with the cross-
 750 sectional area dA and with a liquid stream $Lf(t)dt$. Here, $f(t)$ is the liquid residence time func-
 751 tion that describes, how much time different fluid elements have resided on the tray quantita-
 752 tively.⁹¹ Using assumption (i), the residence time of each stream is given by

$$t \propto \frac{dA}{Lf(t)dt} \quad (42)$$

753 Similarly, the mean residence time of all streams is

$$\tau \propto \frac{A}{L} \quad (43)$$

754 Since the proportionality constant is the same in Eqs. 42 and 43, the fraction of the total froth
 755 volume on the tray occupied by a differential element is directly proportional to its residence
 756 time and the fraction of the total flow as

$$\frac{dA}{A} = \frac{t}{\tau} f(t) dt \quad . \quad (44)$$

757 Using the assumption (ii) and Eq. 44, one can obtain

$$\frac{dG}{G} = \frac{dA}{A} = \frac{t}{\tau} f(t) dt \quad . \quad (45)$$

758 The mass balance in the elemental volume ($dA \cdot dz$) located at point z (with reference to Fig. 21)
 759 results in

$$L f(t) dt \left\{ \frac{\partial x(z, t)}{\partial z} dz \right\} + dG \{ y(z, t) - y_{in} \} \frac{dz}{Z_1} + K dA dz \{ x(z, t) - \bar{x}(z) \} = 0 \quad . \quad (46)$$

760 The first two terms in the above equation describe the net mass transfer corresponding to liquid
 761 and gas flow, respectively, whereas the last term represents the intermixing of liquid owing to
 762 diffusion in the differential element. This intermixing is assumed to be proportional to the size of
 763 the fluid element. $\bar{x}(z)$ is the space-mean concentration at point z , which is defined as

$$\bar{x}(z) = \int_0^A x(z, t) \frac{dA}{A} = \int_0^\infty x(z, t) \frac{t}{\tau} f(t) dt \quad . \quad (47)$$

764 The mathematical treatment on Eq. 46 to obtain the tray efficiency is described in Appendix D,
 765 which results as

$$E_{MV} = \frac{1 - \int_0^\infty \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt}{\lambda \int_0^\infty \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt} \quad . \quad (48)$$

766 The procedure to calculate the point efficiency is briefly introduced in the AIChE model in Sec-
 767 tion 3.3.1. If the point efficiency is supposed to be constant, then the tray efficiency can be ex-
 768 pressed as

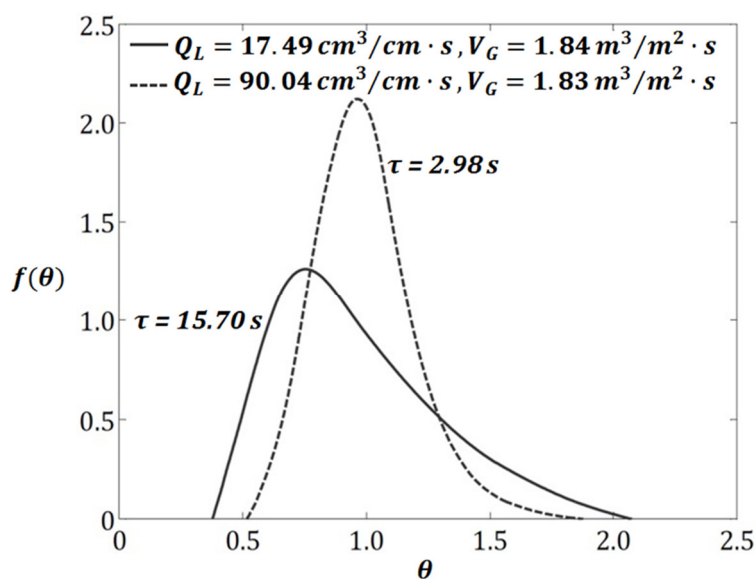
$$\frac{E_{MV}}{E_{OG}} = \frac{1 - \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt}{\lambda E_{OG} \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt} \quad (49)$$

769 As mentioned previously, a cross-check is performed on the tray efficiency by analyzing the
 770 transformation of the model for completely mixed and plug flow cases. The residence time func-
 771 tions are available for the systems with completely mixed and unmixed liquid. By supplying
 772 these functions to Eq. 49, the efficiency for the respective cases of mixing is easy to obtain.⁸⁵

773 The dependency of the tray fractionation efficiency on $f(t)$ and λE_{OG} is evident from Eq. 49. As
 774 far as previous tray models are concerned, liquid mixing in the flow direction is accounted by the
 775 Péclet number. Except for the eddy diffusion model,^{21,58,82} no account of the Péclet number nor-
 776 mal to the flow direction for transverse mixing has been observed. The absence of Péclet number
 777 in this model is automatically compensated by the residence time function, as it also recognizes
 778 the mixing in the flow direction. However, point tracer concentration measurements in stimulus-
 779 response experiments further enable to extract the flow patterns on the trays.^{18,26-28} The cor-
 780 rectness of this model has been justified through the oxygen-stripping studies⁹² on a sieve tray
 781 unit operated with oxygen-rich water and air. The present model slightly over-predicts the effi-
 782 ciency (approximately 5%) due to non-uniform froth conditions at the liquid entrance.⁷³

783 There is a severe lack of data concerning the residence time function of liquid on cross-flow
 784 trays. Foss et al.⁷³ conducted the tracer experiments on a rectangular sieve tray that was 36
 785 inches long and 9.5 inches wide. A concentrated solution of salt was used as the tracer. A step
 786 input of the tracer was supplied to the liquid entering the tray. The tracer concentration in the
 787 effluent stream was measured continuously by a conductivity cell.⁸⁵ The residence time func-
 788 tions with their mean residence time at different load conditions are exemplarily presented in
 789 Fig. 22a.⁷³ The curve with the mean residence time of 15.7 s corresponds to liquid flow rate of
 790 17.49 cm³/(cm·s) and gas flow rate of 1.84 m³/(m²·s). Similarly, the curve with the mean resi-
 791 dence time of 2.98 s corresponds to liquid and gas load of 90.04 cm³/(cm·s) and 1.83 m³/(m²·s),

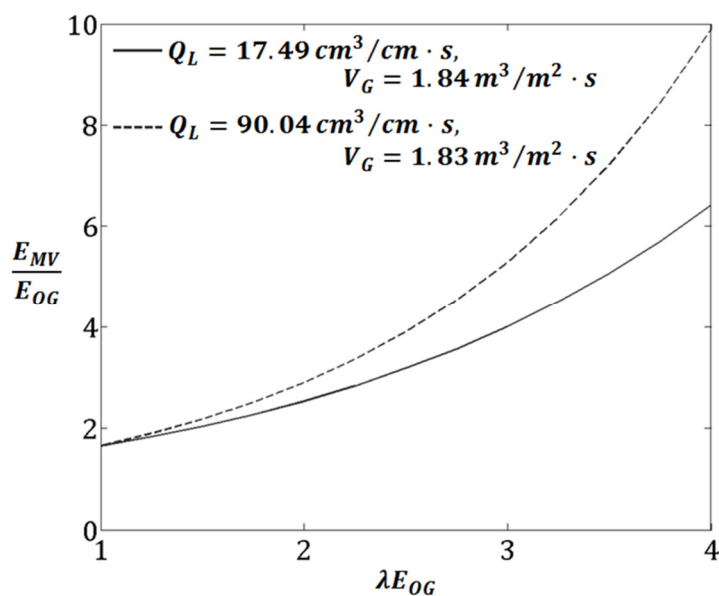
792 respectively. The liquid and gas flow rates are mentioned here with respect to the width and the
 793 active area of the tray, respectively.



794

795

(a)



796

797

(b)

798 **Fig. 22.** (a) Residence time function at the tray outlet and (b) tray efficiency predictions by the
 799 RTD model.

800 Since the time scale of these functions vary from each other, their comparison is only possible by
 801 normalizing their time scale with the corresponding mean time. The occurrence of the lower

802 mean residence time at higher liquid flow rate and vice-versa at constant gas flow is obvious.
803 The spreading of these curves denotes the level of liquid mixing on the tray in the flow direction.
804 The higher the momentum of the liquid, the lower is its axial or longitudinal mixing. Apart from
805 this, the position of the peak of these curves relative to their mean is very important for the di-
806 agnosis of the tray functioning. For instance, a distribution that peaks before its mean indicates
807 the liquid short-circuiting or bypassing.⁷³ These functions are supplied to Eq. 49 to calculate the
808 ratio of the tray and the point efficiencies at different λE_{OG} , as shown in Fig. 22b. This computa-
809 tion is intended only for highlighting the effects of flow and mixing patterns via distribution
810 function on the tray efficiency. Further, the unavailability of the slope of the VLE curve forces to
811 assume a certain value for λE_{OG} since the point efficiency is also supposed to be constant. The
812 separation performance of the tray with higher liquid flow is better than the other case. This is
813 straightforward as the tray with lower liquid flow undergoes liquid bypassing, as suggested by
814 the peak position of the distribution. The E_{MV}/E_{OG} values for λE_{OG} less than unity are not shown
815 here deliberately as these RTD functions are ineligible for these values of λE_{OG} . The difference in
816 the performance of these two cases increases with λE_{OG} , which is consistent with results of the
817 previous models.

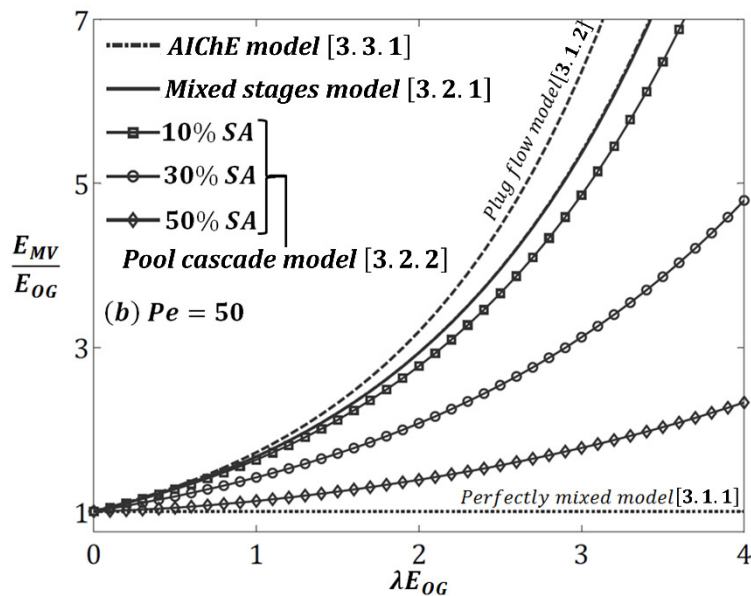
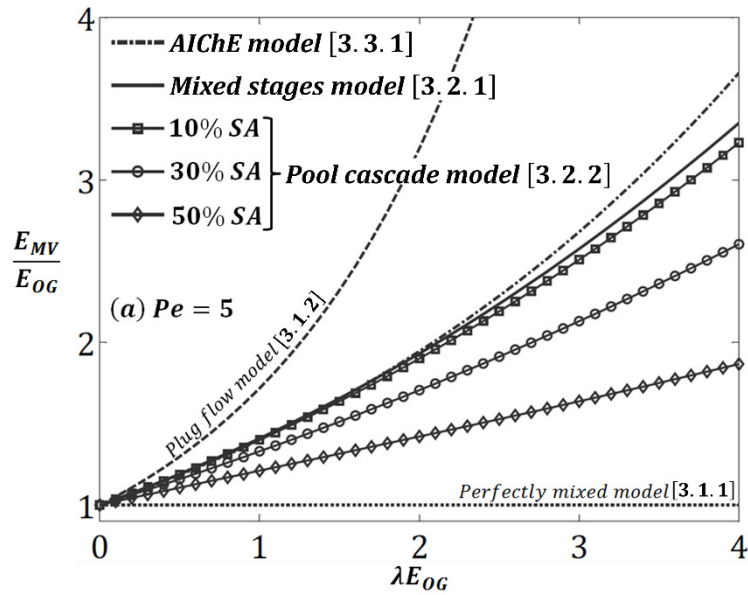
818 A weak point of the RTD studies is that they are unable to uniquely determine the nature,⁹³ as
819 well as the location of the non-ideality. Similar tracer response is possible for different non-
820 idealities at different locations on the tray. However, this approach is the most realistic among
821 the available models since it is unlikely that a number of perfectly mixed pools would actually
822 exist on a tray.⁷³ Furthermore, the concept of eddy diffusion only holds, when there are large
823 number of repetitions of the diffusive mechanism and, is incapable of handling extreme liquid
824 bypassing.⁷³ The RTD model, however, is capable of addressing these possibilities. The feasibility
825 of tracer-response experiments further makes this model a prominent choice for the efficiency
826 predictions, especially in industry.

827

828 4. Comparison of Modeling Schemes

829 In order to compare the results of the existing models, the factors on which these models rely
830 need to be considered. λE_{OG} and Pe appear in almost every model, while the other factors are
831 weir length to diameter ratio,⁵⁸ relative size of active and stagnant regions,⁶⁷ liquid composi-
832 tion,⁵⁸ and residence time function.⁷³ This diversity in factors hinders the straightforward com-
833 parison of the models on a common ground. Thus, an attempt to collate the results from some of
834 the existing methods at arbitrarily selected values of Pe for the usual range of λE_{OG} is demon-
835 strated in Fig. 23a and 23b.

836 The plug flow [3.1.2] and the perfectly mixed [3.1.1] model provide the upper and the lower lim-
837 its of the tray efficiency, respectively. The predictions by the mixed stages model [3.2.1] and the
838 AIChE model [3.3.1] at $Pe = 50$ practically coincide. These models consider the liquid backmix-
839 ing only and are unconcerned towards the stagnant regions due to which the results from the
840 pool cascade model [3.2.2] at $\beta_o = 4$ are also presented. It is obvious that the size of the stagnant
841 regions is proportional to the loss in the tray efficiency. The influence of λE_{OG} and Péclet number
842 on the tray efficiency has been discussed several times in this work. However, this model com-
843 parison is only applicable for the tray assuming uniform liquid flow at the inlet. Apart from this,
844 Bell and Solari⁸⁴ reported that the tray efficiency becomes less than the point efficiency for an
845 inverted parabolic velocity profile of liquid at the inlet (see Fig. 20). The pool cascade model also
846 provides similar observation (not shown here) e.g. the E_{MV}/E_{OG} ratio goes below unity for rela-
847 tive stagnant regions larger than 80% at $Pe = 5$.



848

849

850 **Fig. 23.** Comparison of efficiency predictions from different tray models at (a) $Pe = 5$ and

851 (b) $Pe = 50$.

852 Furthermore, the tray models are summarized in Tab. 4 in terms of their ability to account for
 853 flow and/or mixing patterns. Out of all models, the RTD model is the most realistic one as it is
 854 capable of describing all types of liquid mixing in the flow direction on the tray. The point mean
 855 residence time calculations further reveal the flow profiles on the tray. To make this model bet-
 856 ter, it needs to be upgraded so that it can account for transverse mixing of the liquid and can
 857 differentiate between the effects of different non-idealities on the tray efficiency. A significant
 858 development in the tray efficiency modeling would be the inclusion of possible non-uniform

859 vapor distributions in the model formulation. Further, the ‘Hybrid modeling’ approach combin-
 860 ing experimentally validated CFD and tray efficiency models seems to be a promising alternative
 861 for realistic efficiency predictions. Such hybrid approach could be preferred in the future as ‘vir-
 862 tual experiment’³⁶ compared to real experiments which can be expensive and time consuming.
 863 Besides, the discussed models have been developed for non-reactive systems and hence, it
 864 would be interesting to modify the most prominent ones for the reacting systems.⁹ Lastly, the
 865 tray efficiencies are calculated using the flow conditions at the tray boundaries, i.e. inlet and
 866 outlet, without giving any preference to the flow scenario at intermediate locations (except in
 867 the eddy diffusion model). This is similar to the treatment of distillation trays as black box.
 868 Therefore, an account of the intermediate flow conditions in phenomenological models for
 869 evolving tray efficiencies is another necessity.

870 Tab. 4: Summarization of existing tray models according to their respective account of flow pat-
 871 terns and liquid mixing on the tray. (✓ Acknowledged, ✗ Overlooked)

Model	Liquid mixing		Flow pat- terns	Remarks
	Flow direc- tion	Transverse direction		
3.1.1. Perfectly mixed model	✓		✗	Considers uniform liquid composition over the tray
3.1.2. Plug flow model		✗		Predicts the maximum achievable efficiency
3.1.3. Multi-channel plug flow model		✗	✓	Accounts for liquid channeling only
3.2.1. Mixed stages model	✓	✗	✗	Sensitive to backmixing of liquid only
3.2.2. Pool cascade model	✓	✓	✗	Concerned towards channeling and stagnant zones
3.3.1. AIChE model	✓	✗	✗	Most popular; accounts for liquid backmixing only
3.3.2. Eddy diffusion model	✓	✓	✓	Most all-round model yet computationally expensive
3.4. Non-uniform flow model		✗	✓	Capable of distinguishing between the effects of velocity profiles on tray efficiency
3.5. RTD model	✓	✗	✓	Most realistic model to account for flow patterns and liquid mixing in the flow direction

872 **5. From Experiments to Efficiency Predictions: A Roadmap**

873 One obvious question that remain unanswered is that how to utilize the experimental studies for
874 extracting the inputs required for the mathematical models. The stimulus-response method has
875 been a popular choice to quantify the flow patterns in process equipments, and was preferred by
876 Solari and Bell²⁶ and Schubert et al.¹⁸, while using fibre-optic system and conductivity wire mesh
877 sensor (WMS) respectively. The latter study is favored for the aforementioned purpose due to
878 the availability of data at comparatively high spatial and temporal resolution. In this investiga-
879 tion, two sieve trays with 5% fractional open area were used in an 800 mm diameter column. A
880 WMS, comprising of two orthogonal planes of transmitting and receiving wires, was embedded
881 on one of the trays. The effects of liquid load and outlet weir design on the flow patterns were
882 evaluated through the dispersion of salt (Na_2SO_4) solution used as the tracer. The virtual cross-
883 ing points between axially separated transmitters and receivers in the WMS allow measuring
884 time-dependent tracer concentrations, and hence point liquid residence time distribution. The
885 readers are referred to Schubert et al.¹⁸ for further details on column design, data calibration
886 and flow visualization.

887 The distribution of liquid residence time represents the extent of flow non-idealities in a system.
888 This distribution is opportune as its mathematical processing can lead to determination of the
889 parameters needed in the described models. The point tracer concentrations need to be aver-
890 aged at the tray boundaries to realize the RTD function according to

$$C_{out}(t) = C_{in}(t) \otimes f(t) \quad . \quad (50)$$

891 Here, $C_{in}(t)$ and $C_{out}(t)$ are the tracer concentrations that are mathematically averaged point
892 concentrations for each time step at the tray inlet and outlet, respectively. In this work, the data
893 from the WMS points next to the weirs are avoided to neglect the effect of non-uniform froth at
894 the boundaries⁷³, as well as to account for the flow in the tray bubbling area only. These bounda-
895 ries will be referred as WMS boundaries hereafter. Furthermore, the symbol \otimes refers to the

896 convolution integral, whose calculation is straightforward.^{90,94} The converse of this integral is
 897 called deconvolution, which is challenging and hence requires special approaches.⁹⁴ For this
 898 purpose, several techniques such as Laplace and Fourier methods, flow model fitting, simultane-
 899 ous solution of linear equations, and others have been proposed in the literature.^{90,94-108} The cit-
 900 ed literature also explains the pros and cons of these techniques due to which they are not dis-
 901 cussed here. The model fitting approach is preferred in this work, because of the computational
 902 ease due to the availability of the standard RTD function from the axial dispersion model. The
 903 WMS boundaries permit to use the Gaussian function for the open-open boundary
 904 condition^{90,101,109} as

$$f(t) = \sqrt{\frac{Pe}{4\pi t\tau_h}} \cdot \exp\left\{-\frac{Pe\left(1 - \frac{t}{\tau_h}\right)^2}{4\left(\frac{t}{\tau_h}\right)}\right\} . \quad (51)$$

905 Here, τ_h is the time based on bulk liquid velocity and flow path length, and is called as hydraulic
 906 or space time. Before proceeding further, it is important to focus on the Péclet number in the
 907 above equation. Levenspiel⁹⁰ suggested to refer to this term as an inverse of the vessel disper-
 908 sion number, and strongly objected the usage of the Péclet number. Still, Pe is being used here
 909 due to its popularity and wide acceptance in the chemical reactor engineering. Further, it has
 910 been defined in the literature^{90,91} as

$$Pe = \frac{\text{Movement by bulk flow}}{\text{Movement by longitudinal dispersion}} = \frac{Z_1^2}{D_E \cdot \tau_h} . \quad (52)$$

911 This generalized definition of Pe is apt for the open-open boundary condition. For the closed
 912 system, the mean residence time is the same as the hydraulic time.^{90,91} This is an explanation for
 913 the appearance of the mean residence time in Eq. 23 as proposed in the AIChE manual⁶⁹.

914 The algorithm to obtain the tray RTD function is discussed concisely as following:

915 (i) Compute the response function at the WMS boundaries according to

$$R(t) = \frac{c(t)}{\int_0^{\infty} c(t)dt} \quad . \quad (53)$$

- 916 (ii) Assume the adjustable parameters, i.e. Pe and τ_h , in Eq. 51 and calculate the approx-
 917 imate RTD function.
- 918 (iii) Convolute the inlet response and the RTD function leading to the convoluted func-
 919 tion.
- 920 (iv) Apply the non-linear least-square method to fit the convoluted function with the out-
 921 let response by adjusting the parameters iteratively. This leads to determination of
 922 the RTD function, Pe and τ_h for a good agreement between the actual and the convo-
 923 luted function.¹¹⁰

924 Further, the mean residence time can be obtained from the hydraulic time in the open-open sys-
 925 tem⁹⁰ as

$$\tau = \tau_h \cdot \left(1 + \frac{2}{Pe}\right) \quad , \quad (54)$$

926 while the other definition of τ is given by Eq. D3 in the Appendix D. The residence times obtained
 927 from Eq. 54 and D3 are consistent, which proves the validity of the RTD function as well as of
 928 this algorithm. The rationality of this algorithm can be further justified by the consistency of the
 929 RTD variances according to⁹⁰

$$\sigma^2 = \tau_h^2 \cdot \left(\frac{2}{Pe} + \frac{8}{Pe^2}\right) \quad , \text{ and} \quad (55)$$

$$\sigma^2 = \int_0^{\infty} (t - \tau)^2 \cdot f(t)dt \quad . \quad (56)$$

930 The estimation of the RTD enables computing the relative active and stagnant volumes on the
 931 tray. Duduković and Felder¹¹¹ suggested the tail of the impulse response function, accountable
 932 for the stagnant volume, to be truncated to acquire the active volume. Such truncation is re-
 933 searcher's perception dependent, and can lead to inconsistent fractions. Sahai and Emi¹¹² pro-
 934 posed that any fluid staying in a system for a period longer than twice the mean residence time

935 can be considered as the stagnant or dead volume. Using this theory, the relative stagnant area
936 due to the assumption of uniform froth height can be determined as

$$\phi_d = 1 - \frac{1}{\tau} \left\{ \left(\int_{t=0}^{t=2\tau} f(t) dt \right) \left(\int_{t=0}^{t=2\tau} t \cdot f(t) dt \right) \right\} . \quad (57)$$

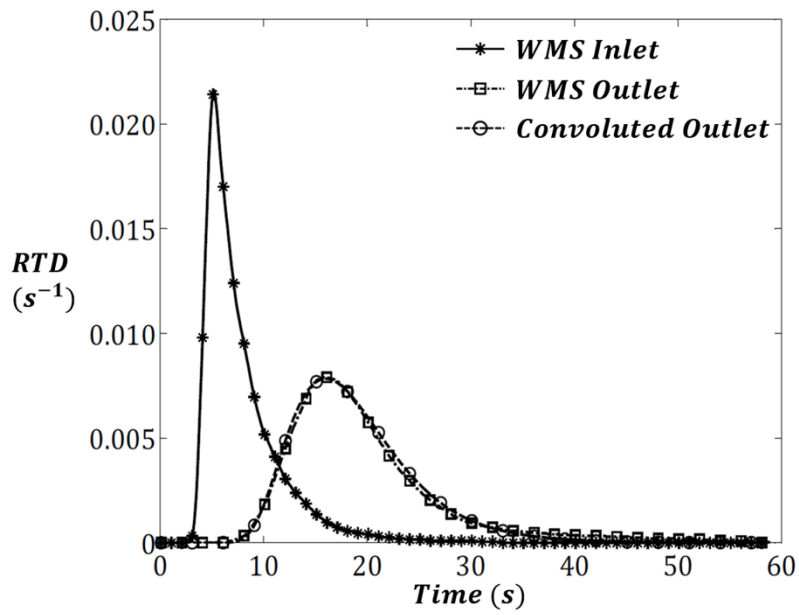
937 With reference to Schubert et al.¹⁸, two different liquid loads, i.e. 2 m³/h and 3 m³/h, during the
938 standard weir operation on a sieve tray at 0.72 Pa^{1/2} F-factor are considered here. The applica-
939 tion of the reported approaches in this section on the experimental data yields the RTD and the
940 associated parameters as presented in Fig. 24. A good agreement between the convoluted func-
941 tion and the WMS outlet response (shown for the lower liquid flow) is apparent in Fig. 24a. On
942 comparison with higher liquid flow on the tray, lower liquid load exhibits higher residence time,
943 smaller Péclet number and larger percentage of liquid stagnancy, yet there is little difference in
944 their numerical values (refer Fig. 24b).

945

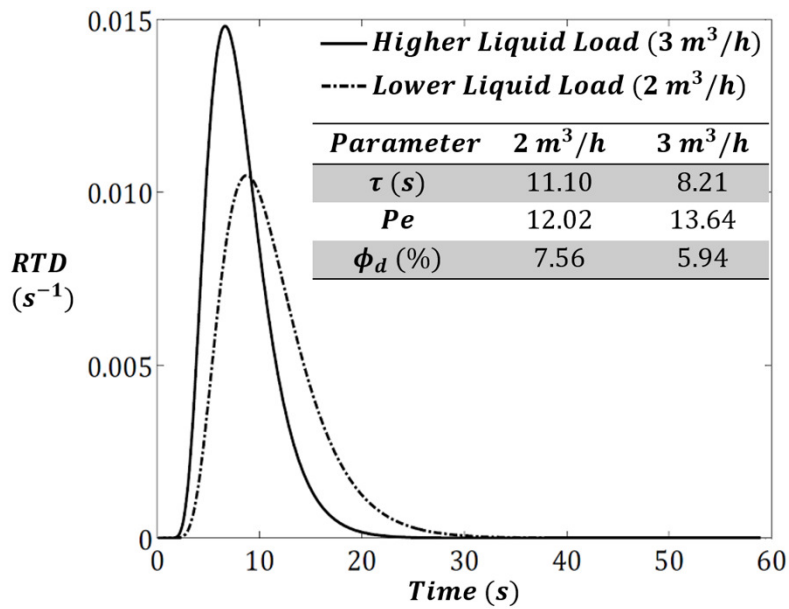
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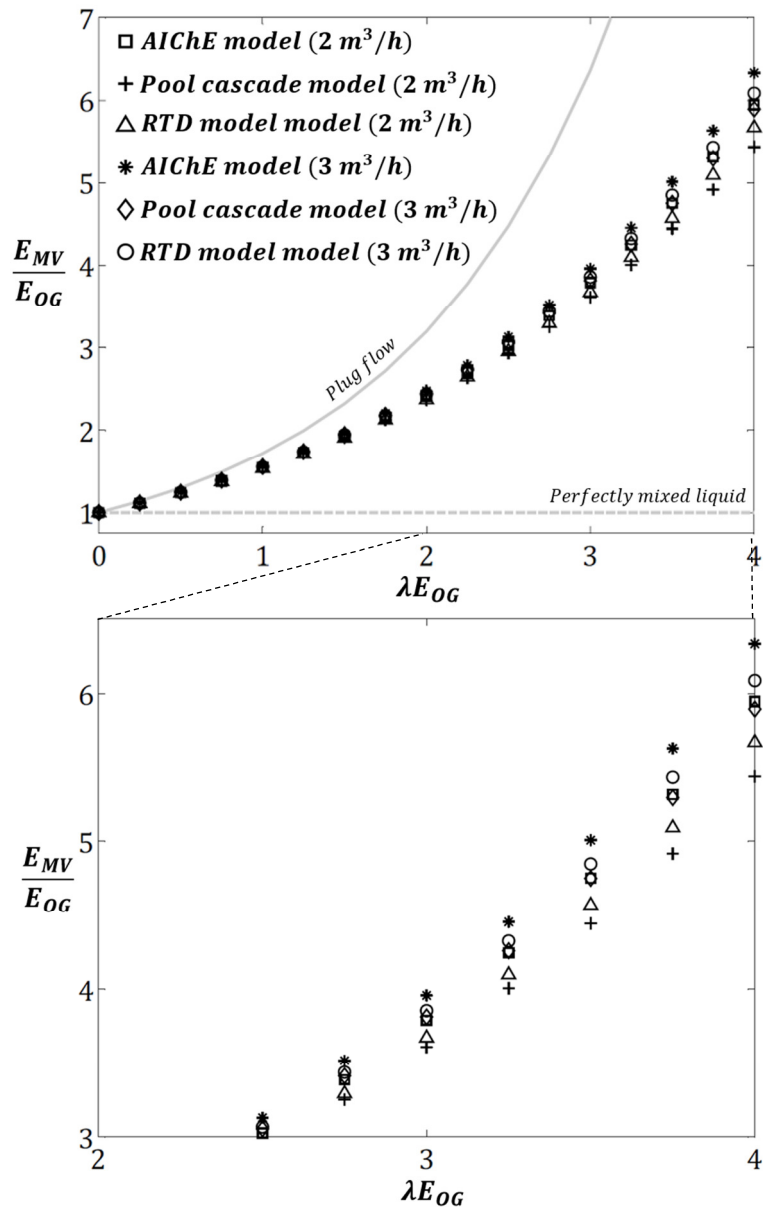


(a)



(b)

Fig. 24. (a) Response and convoluted function at the WMS boundaries for lower liquid flow and (b) tray RTD functions with associated parameters.



957

958
959
960

Fig. 25. Efficiency predictions based on the WMS data for different liquid loads

961 The RTD model, the AIChE model and the pool cascade model are used to predict the tray effi-
 962 ciency for the assumed λE_{OG} . The mixed pool model is the limiting case of the pool cascade mod-
 963 el for no stagnant liquid, while the eddy diffusion model requires serious computational effort
 964 due to which these models are excluded from this analysis. Due to little difference in the para-
 965 metric values for the considered liquid loads as in Fig. 24b, the model predictions are consistent
 966 with each other for the values of λE_{OG} upto 2 as observed in Fig. 25. A slight difference in the
 967 separation efficiency becomes noticeable for the λE_{OG} greater than 2, where the tray efficiency is
 968 relatively higher for the higher liquid flow. This justifies that higher Péclet number and smaller

969 stagnant regions are beneficial for the tray efficiency, and vice-versa. With reference to the RTD
970 model that is considered as the most realistic and accurate model available, the AIChE model
971 and the pool cascade model slightly overpredicts and underpredicts the tray efficiency, respec-
972 tively. The overprediction of the tray efficiency by the AIChE model is upto 5%, while the effi-
973 ciency underprediction in case of the pool cascade model is upto 4% for the given range of λE_{OG} .
974 Further, the predictions from the pool model correspond to $\beta_o = 4$, which on adjustment (as in
975 Fig. 13) could predict the efficiency closer to the RTD model. Thus, an example on the extraction
976 of the fluid dynamics data from experiments and subsequent realization of the efficiency predic-
977 tions from mathematical models is hereby demonstrated.

978

979 **6. Concluding Remarks and Perspective**

980 Flow and mixing patterns on cross-flow trays are significant for their separation efficiency. The
981 distillation trays can no longer be perceived as black-box, as technological advances in meas-
982 urement and imaging techniques have been successful in quantifying the flow on them at high
983 spatial and temporal resolution. The experimental data needs to be processed using mathemati-
984 cal models for calculating the tray efficiency. The development of new tray efficiency models or
985 improvements in the existing ones is desired parallel to advances in CFD modeling and meas-
986 urements. In order to make these columns cost and energy efficient, an improvement in mass-
987 transfer characteristics of column trays through design modification and revamping seems to be
988 a potential nomination. This is possible after their efficiency is accounted accurately. This serves
989 as a motivation for further advancements in the efficiency modeling so that a better interpreta-
990 tion regarding the tray functioning becomes available. Further, a hybrid approach i.e. using
991 mathematical models supplemented with the fluid dynamics information from experimentally
992 validated CFD models, could be preferred in the future for tray efficiency predictions. Therefore,
993 the experimental and the simulation studies intended for column tray flow patterns have been
994 reviewed in this work. In particular, a comprehensive evaluation of the tray efficiency prediction

995 models has been presented by stating their formulation, strengths, weaknesses and associated
996 analysis. Also, the dependence of the tray efficiency on system and flow properties has been
997 discussed. Furthermore, a concise algorithm concerning the processing and utilization of the
998 experimental data in tandem with mathematical models has been proposed. This work is anti-
999 cipated to provide an insight on the tray efficiency modeling, and aims at invigorating the research
1000 in tray columns for future developments.

1001

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1005

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1008

1009 **8. Nomenclature**

1010	A	Cross-sectional area of froth perpendicular to the flow direction (m^2)
1011	A_b	Bubbling or perforated area of the tray (m^2)
1012	b	Slope of the VLE line (-)
1013	$C_{in}(t)$	Time-dependent tracer concentration at the tray (or WMS) inlet (mol/m^3)
1014	$C_{out}(t)$	Time-dependent tracer concentration at the tray (or WMS) outlet (mol/m^3)
1015	$c(t)$	Time-dependent tracer concentration (mol/m^3)
1016	c_1, c_2	Constants in Appendix B (-)
1017	D	Tray diameter (m)
1018	D_E	Eddy diffusion coefficient (m^2/s)
1019	E_{ML}	Liquid-side Murphree tray efficiency (-)

1020	E_{MV}	Vapor or gas-side Murphree tray efficiency (-)
1021	E_o	Overall column efficiency (-)
1022	E_{OG}	Vapor or gas-side point efficiency (-)
1023	$f(t)$	Residence time function (s^{-1})
1024	G	Gas flow rate (kmol/s)
1025	G'	Gas flow rate per tray bubbling area (kmol/($m^2 \cdot s$))
1026	h_F	Froth height (m)
1027	k	Number of channels in Stichlmair's model (-)
1028	K	Diffusion coefficient based on the size of the fluid element in the RTD model
1029		(kmol/($m^3 \cdot s$))
1030	L	Liquid flow rate (kmol/s)
1031	L'	Liquid flow rate per unit weir length (kmol/($m \cdot s$))
1032	m	Tray number (-)
1033	N_{ac}	Actual number of trays in the column (-)
1034	N_{eq}	Number of equilibrium stages in the column (-)
1035	n	Number of pools in the flow direction (-)
1036	\dot{n}	Dimensionless distance normal to the column wall (-)
1037	Pe	Péclet number ($= Z_1^2 / (D_E \cdot \tau)$) (-)
1038	$\dot{P}e$	Péclet number denoting the three-dimensional eddy mixing (-)
1039	p	Arbitrary point on the tray (-)
1040	Q	Volumetric flow rate of liquid (m^3/s)
1041	Q_L	Volumetric flow rate of liquid per tray width (m^2/s)
1042	q_s	Normalized slip velocity at the wall (-)
1043	$q(\xi)$	Normalized velocity profile function (-)
1044	$R(t)$	Response function (s^{-1})
1045	r_1, r_2	Roots of the differential equation in Appendix B (-)
1046	s	Non-dimensional distance in the flow direction from the inlet weir (-)

1047	T	Parameter used in Appendix A (-)
1048	t	Time (s)
1049	U	Parameter used in Appendix A (-)
1050	V_f	Average froth velocity (m/s)
1051	V_G	Gas velocity (m/s)
1052	W	Weir length (m)
1053	w	Distance from the tray centerline perpendicular to the flow direction (m)
1054	w'	Normalized distance from the tray centerline perpendicular to the flow direction
1055		(= z/D) (-)
1056	X	Parameter used in Appendix B (-)
1057	x	Composition (mole fraction) of the volatile component in the liquid phase (-)
1058	x'	Composition (mole fraction) of the volatile component in the liquid phase in the
1059		side mixers (-)
1060	x_e^*	Liquid composition in equilibrium with the incoming vapor (-)
1061	x_m	Composition of liquid leaving the tray (-)
1062	x_{+m}	Liquid composition at the inlet weir (-)
1063	x_{m1}	Liquid composition at the inlet of the retrograde flow zone (-)
1064	x_{m2}	Mixing cup average composition of liquid leaving the retrograde flow zone (-)
1065	x_m^*	Liquid composition in equilibrium with vapor leaving the tray (-)
1066	x_{m-1}	Composition of liquid entering the tray (-)
1067	$\bar{x}(z)$	Space mean composition of liquid at point z (-)
1068	y	Composition (mole fraction) of the volatile component in the vapor phase (-)
1069	y'	Composition (mole fraction) of the volatile component in the vapor phase in the
1070		side mixers (-)
1071	y_m	Composition of vapor leaving the tray (-)
1072	y_m^*	Composition of vapor in equilibrium with liquid leaving the tray (-)
1073	y_{in}	Composition of vapor entering the tray (-)

1074	y_p	Composition of vapor at point p on the tray (-)
1075	y_p^*	Composition of vapor in equilibrium with liquid at point p on the tray (-)
1076	y_2	Composition of vapor leaving the froth element in the AIChE model (-)
1077	Z_1	Flow path length (m)
1078	z	Distance from inlet weir in the flow direction (m)
1079	z'	Normalized distance from inlet weir in the flow direction ($= z/D$) (-)

1080

1081 **Subscripts**

1082	a	Active region on the tray
1083	d	Stagnant region on the tray
1084	f	Froth
1085	h	Hydraulic
1086	i	Channel index in the multi-channel plug flow model, index for main line mixers in
1087		the pool cascade model
1088	in	Inlet
1089	j	Index for pools and side mixers in the mixed stages model and the pool cascade
1090		model respectively
1091	m	m^{th} tray
1092	$mean$	Mean or average
1093	w	w - direction
1094	z	z - direction

1095

1096 **Superscript**

1097	*	Equilibrium
------	---	-------------

1098 **Greek Letters**

1099	β	Fraction of liquid that circulates between main line mixer and side mixer (-)
1100	β_o	Empirical fitting parameter in the pool cascade model (-)
1101	γ	Parameter used in the plug flow model (-)
1102	δ	Central tray area with forward flow per total tray area (-)
1103	η	Parameter used in the AIChE model (-)
1104	θ	Non-dimensional time (= t/τ) (-)
1105	λ	Stripping factor (-)
1106	ξ	Non-dimensional distance from the tray centerline orthogonal to the flow direction (-)
1107		
1108	ρ_L	Clear liquid density (kmol/m ³)
1109	ρ_F	Froth density (= volume of liquid/froth volume) (-)
1110	σ^2	Variance of the RTD function (s ²)
1111	τ	Mean residence time of the liquid on the tray (s)
1112	τ_h	Hydraulic or space time (= volume of the system/volumetric flow rate) (s)
1113	ϕ_a	Relative volume of the active region in the pool cascade model (-)
1114	ϕ_d	Relative volume of the stagnant region in the pool cascade model (-)
1115	ψ	Stream function (m ² /s)
1116	ψ_o	Stream function value at the column wall (m ² /s)
1117	ω	Fraction of the recycled liquid as retrograde flow (-)

1118

1119 **Abbreviations**

1120	<i>AIChE</i>	American Institute of Chemical Engineers
1121	<i>CFD</i>	Computational fluid dynamics
1122	<i>LES</i>	Large eddy simulation

1123	<i>MDF</i>	Maldistribution factor
1124	<i>RTD</i>	Residence time distribution
1125	<i>SA</i>	Stagnant area
1126	<i>VLE</i>	Vapor-liquid equilibrium
1127	<i>VOF</i>	Volume of fluid
1128	<i>WMS</i>	Wire mesh sensor
1129	<i>2D</i>	Two-dimensional
1130	<i>3D</i>	Three-dimensional

1131

1132 **Appendix (A)**

1133 For plug flow of the liquid, the pool model transforms to

$$E_{MV} = \left[\left(1 + \frac{\phi_a \lambda E_{OG}}{n} \right)^n - 1 \right] / \lambda \quad . \quad (21)$$

1134 Taking $\phi_a \lambda E_{OG} = T$ and $U = n/T$ (used later) for simplicity, the above equation becomes

$$E_{MV} = \left[\left(1 + \frac{T}{n} \right)^n - 1 \right] / \lambda \quad . \quad (A1)$$

1135 For infinite number of pools, $\lim_{n \rightarrow \infty} \left(1 + \frac{T}{n} \right)^n$ needs to be calculated as

$$\lim_{n \rightarrow \infty} \left(1 + \frac{T}{n} \right)^n = \lim_{n \rightarrow \infty} \left\{ \left(1 + \frac{1}{n/T} \right)^{n/T} \right\}^T = \lim_{U \rightarrow \infty} \left\{ \left(1 + \frac{1}{U} \right)^U \right\}^T \quad . \quad (A2)$$

1136 Using the binomial expansion, one can write

$$\begin{aligned} \left(1 + \frac{1}{U} \right)^U &= {}^U C_0 \cdot 1^U \cdot (1/U)^0 + {}^U C_1 \cdot 1^{U-1} \cdot (1/U)^1 + {}^U C_2 \cdot 1^{U-2} \cdot (1/U)^2 + \dots \\ &= 1 + 1 + \frac{U-1}{2U} + \frac{(U-1)(U-2)}{6U^2} + \dots = 1 + 1 + \frac{1}{2} - \frac{1}{2U} + \frac{(1-1/U)(1-2/U)}{6} + \dots \quad (A3) \end{aligned}$$

1137 The application of the limit in Eq. A3 provides

$$\lim_{U \rightarrow \infty} \left(1 + \frac{1}{U}\right)^U = 1 + 1 + \frac{1}{2} + \frac{1}{6} + \dots = e^1 \quad \text{(Maclaurin's series expansion of the exponential function).} \quad (\text{A4})$$

1138 Using Eqs. A1 to A4, it is possible to write Eq. 21 as

$$E_{MV} = \frac{\exp(\phi_a \lambda E_{OG}) - 1}{\lambda} . \quad (\text{22})$$

1139

1140 **Appendix (B)**

1141 The mass balance over the froth element in the AIChE model generates

$$\frac{1}{Pe} \frac{d^2 x}{ds^2} - \frac{dx}{ds} - \lambda E_{OG} (x - x_e^*) = 0 . \quad (\text{27})$$

1142 By assuming $X = x - x_e^*$, Eq. 27 becomes

$$X'' - Pe X' - \lambda E_{OG} Pe X = 0 . \quad (\text{B1})$$

1143 The solution of Eq. B1 is given by

$$r^2 - Pe.r - Pe.\lambda E_{OG} = 0 , \quad (\text{B2})$$

$$r_1, r_2 = \frac{Pe \pm \sqrt{Pe^2 + 4Pe \lambda E_{OG}}}{2} , \text{ and} \quad (\text{B3})$$

$$X = c_1 e^{r_1 s} + c_2 e^{r_2 s} . \quad (\text{B4})$$

1144 Here c_1 and c_2 are the constants while r_1 and r_2 are the roots of the differential equation. The

1145 application of the boundary conditions (Eqs. 28 and 29) to Eq. B4 gives

Boundary condition 1: $X(1) = x_m - x_e^* = c_1 e^{r_1} + c_2 e^{r_2}$ and (B5)

Boundary condition 2: $X'(1) = c_1 r_1 e^{r_1} + c_2 r_2 e^{r_2} = 0$. (B6)

1146 Solving the last three equations for c_1 and c_2 , Eq. B7 is obtained as

$$\frac{x - x_e^*}{x_m - x_e^*} = \frac{\exp\{(\eta + Pe)(s - 1)\}}{1 + \frac{\eta + Pe}{\eta}} + \frac{\exp\{\eta(1 - s)\}}{1 + \frac{\eta}{\eta + Pe}} \quad (B7)$$

where $\eta = \frac{Pe}{2} \left(\sqrt{1 + \frac{4\lambda E_{OG}}{Pe}} - 1 \right)$. (31)

1147 Earlier, it has been stated that

$$y_2 - y_{in} = m(x - x_e^*)E_{OG} \quad (B8)$$

1148 Applying Eq. B8 and considering a constant vapor load of uniform composition at the tray inlet

1149 permits to formulate the tray efficiency as

$$y_m - y_{in} = \int_0^1 (y_2 - y_{in}) ds = mE_{OG} \int_0^1 (x - x_e^*) ds \quad (B9)$$

$$E_{MV} = \frac{y_m - y_{in}}{y_m^* - y_{in}} = \frac{mE_{OG} \int_0^1 (x - x_e^*) ds}{m \int_0^1 (x_m - x_e^*) ds} \quad , \text{ and} \quad (B10)$$

$$\frac{E_{MV}}{E_{OG}} = \frac{\int_0^1 (x - x_e^*) ds}{\int_0^1 (x_m - x_e^*) ds} \quad (B11)$$

1150 The integration on Eq. B11 using Eq. B7 result in

$$\frac{E_{MV}}{E_{OG}} = \frac{1 - \exp\{-(\eta + Pe)\}}{(\eta + Pe) \left(1 + \frac{\eta + Pe}{\eta}\right)} + \frac{\exp(\eta) - 1}{\eta \left(1 + \frac{\eta}{\eta + Pe}\right)} \quad (30)$$

1151

1152 **Appendix (C)**

1153 The mass balance over the froth element in the eddy diffusion model provides

$$D_E h_f \rho_L \rho_f \left(\frac{\partial^2 x}{\partial z^2} + \frac{\partial^2 x}{\partial w^2} \right) - L'_z \frac{\partial x}{\partial z} - L'_w \frac{\partial x}{\partial w} - x \left(\frac{\partial L'_z}{\partial z} + \frac{\partial L'_w}{\partial w} \right) - G' \{y(z, w) - y_{in}\} = 0 \quad . \quad (32)$$

1154 The equation of continuity is

$$\frac{\partial L'_z}{\partial z} + \frac{\partial L'_w}{\partial w} = 0 \quad . \quad (C1)$$

1155 The application of Eq. C1 transforms Eq. 32 as

$$D_E h_f \rho_L \rho_f \left(\frac{\partial^2 x}{\partial z^2} + \frac{\partial^2 x}{\partial w^2} \right) - L'_z \frac{\partial x}{\partial z} - L'_w \frac{\partial x}{\partial w} - G' (y(z, w) - y_{in}) = 0 \quad . \quad (C2)$$

1156 The liquid flow rates that are normal to the directions z and w , i.e. L'_z and L'_w , respectively, are
 1157 replaced by stream function. This function represents a constant liquid flow with respect to the
 1158 tray centerline. The equations defined for this purpose are

$$L'_z = h_f \rho_L \rho_f \frac{\partial \psi}{\partial w} \quad , \quad (C3)$$

$$L'_w = -h_f \rho_L \rho_f \frac{\partial \psi}{\partial z} \quad , \text{ and} \quad (C4)$$

$$L = 2h_f \rho_L \rho_f \psi_o \quad , \quad (C5)$$

1159 where ψ is the stream function that is measured from the centerline of the tray (it is zero at the
 1160 centerline) and ψ_o is the stream function at the column wall (arbitrarily chosen).

1161 The definitions used for E_{OG} and Pe in this model are

$$E_{OG} = \frac{y(z, w) - y_{in}}{y^* - y_{in}} = \frac{y(z, w) - y_{in}}{m(x - x_e^*)} \quad , \text{ and} \quad (C6)$$

$$Pe = \frac{DL}{h_f \rho_L \rho_f W D_E} \quad (C7)$$

1162 Further, the directional variables are normalized by the tray diameter as

$$z' = \frac{z}{D} \quad , \text{ and} \quad (C8)$$

$$w' = \frac{w}{D} \quad . \quad (C9)$$

1163 The application of Eqs. C3 to C9 in Eq. C2 produces Eq. 33 as

$$\frac{1}{Pe} \left(\frac{\partial^2 x}{\partial z'^2} + \frac{\partial^2 x}{\partial w'^2} \right) - \frac{W}{2D\psi_o} \left(\frac{\partial \psi}{\partial w'} \frac{\partial x}{\partial z'} - \frac{\partial \psi}{\partial z'} \frac{\partial x}{\partial w'} \right) - \frac{\lambda E_{OG} W D (x - x_e^*)}{A_b} = 0 \quad . \quad (33)$$

1164

1165 **Appendix (D)**

1166 The material balance over the elemental volume in the RTD model results in

$$Lf(t)dt \left\{ \frac{\partial x(z,t)}{\partial z} dz \right\} + dG \{y(z,t) - y_{in}\} \frac{dz}{Z_1} + KdAdz \{x(z,t) - \bar{x}(z)\} = 0 \quad . \quad (46)$$

1167 Using Eq. 45 to eliminate dA and dG , the usual definitions of point efficiency, stripping factor and

1168 linear VLE relationship, Eq. 47 and assuming $s = z/Z_1$, the above equation becomes

$$f(t) \left[\frac{dx(s,t)}{ds} + \lambda E_{OG} \frac{t}{\tau} \{x(s,t) - x_e^*\} + \frac{KAZ_1 t}{L} \left\{ x(s,t) - \int_0^\infty x(s,t) \frac{t}{\tau} f(t) dt \right\} \right] dt = 0 \quad . \quad (D1)$$

1169 Eq. D1 is integrated over time to account for all fluid elements as

$$\int_0^\infty f(t) \left[\frac{dx(s,t)}{ds} + \lambda E_{OG} \frac{t}{\tau} \{x(s,t) - x_e^*\} + \frac{KAZ_1 t}{L} \left\{ x(s,t) - \int_0^\infty x(s,t) \frac{t}{\tau} f(t) dt \right\} \right] dt = 0 \quad . \quad (D2)$$

1170 The mean residence time is defined as

$$\tau = \int_0^{\infty} t f(t) dt \quad . \quad (D3)$$

1171 Using Eq. D3, Eq. D2 transforms to

$$\int_0^{\infty} f(t) \left[\frac{dx(s, t)}{ds} + \lambda E_{OG} \frac{t}{\tau} \{x(s, t) - x_e^*\} \right] dt = 0 \quad . \quad (D4)$$

1172 Since $0 < t < \infty$ and $f(t) \geq 0$, it is appropriate to write the above equation as

$$\frac{dx(s, t)}{ds} + \lambda E_{OG} \frac{t}{\tau} \{x(s, t) - x_e^*\} = 0 \quad . \quad (D5)$$

1173 Eq. D5 can be solved by the method of separation of variables. Its solution and boundary condi-

1174 tion at the inlet are straightforward and can be easily understood from Eq. D6 as

$$\frac{x(s, t) - x_e^*}{x_{m-1} - x_e^*} = \exp(-\lambda E_{OG} s t / \tau) \quad . \quad (D6)$$

1175 The Murphree efficiency for the liquid-side is

$$E_{ML} = \frac{x_m - x_{m-1}}{x_m^* - x_{m-1}} \quad . \quad (D7)$$

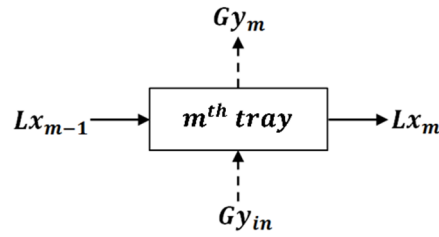
1176 The average composition of liquid exiting the tray can be found using Eq. D6 as

$$x_m = \int_0^{\infty} x(1, t) f(t) dt = x_e^* + (x_{m-1} - x_e^*) \int_0^{\infty} \exp(-\lambda E_{OG} t / \tau) f(t) dt \quad . \quad (D8)$$

1177 The only information required to relate Eq. D8 and Eq. D7 is x_m^* , which can be acquired by fol-

1178 lowing the material balance over the whole tray (refer Fig. D1) as

$$L(x_m - x_{m-1}) = G(y_{in} - y_m) = mG(x_e^* - x_m^*) \quad . \quad (D9)$$



1179

1180

Fig. D1. Material balance over the tray boundaries.

1181

The final expression for the tray efficiency is derived using Eqs. D7 to D9 as

$$E_{ML} = \frac{1 - \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt}{1 - \frac{1}{\lambda} \{1 - \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt\}} \quad (D10)$$

1182

Following a similar procedure, the vapor-side tray efficiency can be arranged as

$$E_{MV} = \frac{1 - \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt}{\lambda \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt} \quad (D11)$$

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1184 References

1185

1. Olujić Ž, Kaibel B, Jansen H, Rietfort T, Zich E, Frey G. Distillation column internals/configurations for process intensification. *Chemical Biochemical Engineering Quarterly*. 2003;17(4):301-309.

1186

1188

2. Górak A, Sorensen E. *Distillation: fundamentals and principles*. Academic Press; 2014.

1189

3. Kister HZ. *Distillation design*. McGraw-Hill New York; 1992.

1190

4. Masoumi ME, Kadkhodaie S. Optimization of energy consumption in sequential distillation column. *World Academy of Science, Engineering and Technology, International Journal of Chemical, Molecular, Nuclear, Materials and Metallurgical Engineering*. 2012;6(1):55-59.

1191

1192

1193

1194

5. Lockett MJ. *Distillation tray fundamentals*. Cambridge University Press; 1986.

1195

6. Murphree E. Rectifying column calculations. *Industrial and Engineering Chemistry*. 1925;17(7):747-750.

1196

- 1197 7. Brambilla A. The effect of vapour mixing on efficiency of large diameter distillation
1198 plates. *Chemical Engineering Science*. 1976;31(7):517-523.
- 1199 8. Onda K, Sada E, Takahashi K, Mukhtar SA. Plate and column efficiencies of continuous
1200 rectifying columns for binary mixtures. *AIChE Journal*. 1971;17(5):1141-1152.
- 1201 9. Fisher KS, Rochelle GT. Effect of mixing on efficiencies for reactive tray contactors. *AIChE*
1202 *Journal*. 2002;48(11):2537-2544.
- 1203 10. Stichlmair J, Ulbrich S. Liquid channelling on trays and its effect on plate efficiency.
1204 *Chemical Engineering and Technology*. 1987;10(1):33-37.
- 1205 11. Hausen H. Zur definition des austauschgrades von rektifizierböden bei zwei-und
1206 dreistoff-gemischen. *Chemie Ingenieur Technik*. 1953;25(10):595-597.
- 1207 12. Standart G. Generalized definition of a theoretical plate or stage of contacting equipment.
1208 *Chemical Engineering Science*. 1965;20(6):611-622.
- 1209 13. Holland CD, McMahon KS. Comparison of vaporization efficiencies with Murphree-type
1210 efficiencies in distillation—I. *Chemical Engineering Science*. 1970;25(3):431-436.
- 1211 14. Holland CD. *Fundamentals of multicomponent distillation*. McGraw-Hill; 1981.
- 1212 15. Jaćimović BM, Genić SB. Normalized efficiency for stagewise operations. *Industrial and*
1213 *Engineering Chemistry Research*. 2011;50(12):7437-7444.
- 1214 16. Jaćimović BM, Genić SB. Tray efficiency versus stripping factor. *Industrial and*
1215 *Engineering Chemistry Research*. 2011;50(12):7445-7451.
- 1216 17. Nandakumar K, Chuang KT. Tray columns: performance. *Hydrocarbon Processing*.
1217 2000;65(43):1140-1145.
- 1218 18. Schubert M, Piechotta M, Beyer M, Schleicher E, Hampel U, Paschold J. An imaging
1219 technique for characterization of fluid flow pattern on industrial-scale column sieve
1220 trays. *Chemical Engineering Research and Design*. 2016;111:138-146.
- 1221 19. Müller EA, Cavero A, Antonio Estévez L. Improving flow patterns in a distillation tray by
1222 modifying downcomer apron shape. *Chemical Engineering Communications*.
1223 1988;74(1):195-208.

- 1224 20. Lockett MJ, Safekourdi A. The effect of the liquid flow pattern on distillation plate
1225 efficiency. *Chemical Engineering Journal*. 1976;11(2):111-121.
- 1226 21. Porter KE, Lockett MJ, Lim CT. The effect of liquid channeling on distillation plate
1227 efficiency. *Transactions of the Institution of Chemical Engineers*. 1972;50(2):91-101.
- 1228 22. Sohlo J, Kinnunen S. Dispersion and flow phenomena on a sieve plate. *Transactions of the*
1229 *Institution of Chemical Engineers*. 1977;55:71-73.
- 1230 23. Porter KE, Yu KT, Chambers S, Zhang MQ. Flow patterns and temperature profiles on a
1231 2.44 m diameter sieve tray. *Chemical Engineering Research and Design*. 1992;70(A):489-
1232 500.
- 1233 24. Li Y, Wang L, Yao K. New technique for measuring fluid flow patterns on a multiple
1234 downcomer tray. *Industrial and Engineering Chemistry Research*. 2007;46(9):2892-2897.
- 1235 25. Biddulph MW, Bultitude DP. Flow characteristics of a small-hole sieve tray. *AIChE*
1236 *Journal*. 1990;36(12):1913-1916.
- 1237 26. Solari RB, Bell RL. Fluid flow patterns and velocity distribution on commercial-scale
1238 sieve trays. *AIChE Journal*. 1986;32(4):640-649.
- 1239 27. Bell RL. Experimental determination of residence time distributions on commercial scale
1240 distillation trays using a fiber optic technique. *AIChE Journal*. 1972;18(3):491-497.
- 1241 28. Bell RL. Residence time and fluid mixing on commercial scale sieve trays. *AIChE Journal*.
1242 1972;18(3):498-505.
- 1243 29. Yu KT, Huang J, Li JL, Song HH. Two-dimensional flow and eddy diffusion on a sieve tray.
1244 *Chemical Engineering Science*. 1990;45(9):2901-2906.
- 1245 30. Liu C, Yuan X, Yu KT, Zhu X. A fluid-dynamic model for flow pattern on a distillation tray.
1246 *Chemical Engineering Science*. 2000;55(12):2287-2294.
- 1247 31. Mehta B, Chuang K, Nandakumar K. Model for liquid phase flow on sieve trays. *Chemical*
1248 *Engineering Research and Design*. 1998;76(7):843-848.
- 1249 32. Krishna R, Van Baten J, Ellenberger J, Higler A, Taylor R. CFD simulations of sieve tray
1250 hydrodynamics. *Chemical Engineering Research and Design*. 1999;77(7):639-646.

- 1251 33. Van Baten J, Krishna R. Modelling sieve tray hydraulics using computational fluid
1252 dynamics. *Chemical Engineering Journal*. 2000;77(3):143-151.
- 1253 34. Gesit G, Nandakumar K, Chuang KT. CFD modeling of flow patterns and hydraulics of
1254 commercial-scale sieve trays. *AIChE Journal*. 2003;49(4):910-924.
- 1255 35. Wang XL, Liu CJ, Yuan XG, Yu K. Computational fluid dynamics simulation of three-
1256 dimensional liquid flow and mass transfer on distillation column trays. *Industrial and
1257 Engineering Chemistry Research*. 2004;43(10):2556-2567.
- 1258 36. Rahimi R, Rahimi MR, Zivdar M. Efficiencies of sieve tray distillation columns by CFD
1259 simulation. *Chemical Engineering and Technology*. 2006;29(3):326-335.
- 1260 37. Noriler D, Meier H, Barros A, Maciel MW. Thermal fluid dynamics analysis of gas-liquid
1261 flow on a distillation sieve tray. *Chemical Engineering Journal*. 2008;136(2):133-143.
- 1262 38. Noriler D, Barros AA, Maciel MRW, Meier HF. Simultaneous momentum, mass, and
1263 energy transfer analysis of a distillation sieve tray using CFD techniques: prediction of
1264 efficiencies. *Industrial and Engineering Chemistry Research*. 2010;49(14):6599-6611.
- 1265 39. Li X, Yang N, Sun Y, Zhang L, Li X, Jiang B. Computational fluid dynamics modeling of
1266 hydrodynamics of a new type of fixed valve tray. *Industrial and Engineering Chemistry
1267 Research*. 2013;53(1):379-389.
- 1268 40. Ping Z, Dan J, Huibo M, Jianhua W. Three-dimensional simulation of liquid flow on a sieve
1269 tray under different inclinations. *Brazilian Journal of Chemical Engineering*.
1270 2014;31(4):905-912.
- 1271 41. Li Q, Li L, Zhang M, Lei Z. Modeling flow-guided sieve tray hydraulics using
1272 computational fluid dynamics. *Industrial and Engineering Chemistry Research*.
1273 2014;53(11):4480-4488.
- 1274 42. Zarei T, Abedini E, Rahimi R, Khorshidi J. Computational fluid dynamics on the
1275 hydrodynamic characteristics of the conical cap tray. *Korean Journal of Chemical
1276 Engineering*. 2017;34(4):969-976.

- 1277 43. Bennett D, Agrawal R, Cook P. New pressure drop correlation for sieve tray distillation
1278 columns. *AIChE Journal*. 1983;29(3):434-442.
- 1279 44. Colwell CJ. Clear liquid height and froth density on sieve trays. *Industrial and Engineering
1280 Chemistry Process Design and Development*. 1981;20(2):298-307.
- 1281 45. Schultes M. Research on mass transfer columns: passé? *Chemical Engineering and
1282 Technology*. 2013;36(9):1539-1549.
- 1283 46. Sakata M, Yanagi T. Performance of a commercial scale sieve tray. Paper presented at:
1284 Institution of Chemical Engineers Symposium Series1979.
- 1285 47. Taylor R. (Di) Still modeling after all these years: a view of the state of the art. *Industrial
1286 and Engineering Chemistry Research*. 2007;46(13):4349-4357.
- 1287 48. Zarei T, Rahimi R, Zivdar M. Computational fluid dynamic simulation of MVG tray
1288 hydraulics. *Korean Journal of Chemical Engineering*. 2009;26(5):1213.
- 1289 49. Rahimi R, Sotoodeh MM, Bahramifar E. The effect of tray geometry on the sieve tray
1290 efficiency. *Chemical Engineering Science*. 2012;76:90-98.
- 1291 50. Jiang S, Gao H, Sun J, Wang Y, Zhang L. Modeling fixed triangular valve tray hydraulics
1292 using computational fluid dynamics. *Chemical Engineering and Processing: Process
1293 Intensification*. 2012;52:74-84.
- 1294 51. Jiang B, Liu P, Zhang L, et al. Hydrodynamics and mass-transfer analysis of a distillation
1295 ripple tray by computational fluid dynamics simulation. *Industrial and Engineering
1296 Chemistry Research*. 2013;52(49):17618-17626.
- 1297 52. Sun J, Luo X, Jiang S, et al. Computational fluid dynamics hydrodynamic analysis of a
1298 cross-orthogonal fixed-valve tray. *Chemical Engineering and Technology*.
1299 2014;37(3):383-391.
- 1300 53. Albadawi A, Donoghue D, Robinson A, Murray D, Delauré Y. Influence of surface tension
1301 implementation in volume of fluid and coupled volume of fluid with level set methods for
1302 bubble growth and detachment. *International Journal of Multiphase Flow*. 2013;53:11-28.

- 1303 54. Malvin A, Chan A, Lau PL. CFD study of distillation sieve tray flow regimes using the
1304 droplet size distribution technique. *Journal of the Taiwan Institute of Chemical Engineers*.
1305 2014;45(4):1354-1368.
- 1306 55. Li X, Cong H, Gao X, Li H. Investigation and simulation on the performance of the elliptical
1307 tray placed in the unconventional “s” shape distillation column. *Journal of the Taiwan*
1308 *Institute of Chemical Engineers*. 2016;60:44-58.
- 1309 56. Zarei T, Rahimi R, Zarei A, Zivdar M. Hydrodynamic characteristic of Conical Cap tray:
1310 Experimental studies on dry and total pressure drop, weeping and entrainment.
1311 *Chemical Engineering and Processing: Process Intensification*. 2013;64:17-23.
- 1312 57. Lockett MM, Dhulesia HA. Murphree Plate Efficiency with Nonuniform Vapour
1313 Distribution. *Chemical Engineering Journal*. 1980;19(3):183-188.
- 1314 58. Safekourdi A. *The effect of liquid flow pattern on distillation plate efficiency* [Doctoral
1315 dissertation], The Victoria University of Manchester; 1975.
- 1316 59. Kirschbaum E. Efficiency of Rectification and Appropriate Path for Liquid Flow.
1317 *Forschung auf dem Gebiete des Ingenieurwesens*. 1934;5:245.
- 1318 60. Lewis Jr WK. Rectification of binary mixtures. *Industrial and Engineering Chemistry*.
1319 1936;28(4):399-402.
- 1320 61. King CJ. *Separation processes*. Courier Corporation; 2013.
- 1321 62. Olujic Z, Van Baak R, Haaring J. Liquid distribution behaviour of conventional and high
1322 capacity structured packings. *Institution of Chemical Engineers*. 2006;152:252-266.
- 1323 63. Kirschbaum E. *Distillation and rectification*. Chemical Publishing Company; 1948.
- 1324 64. Gautreaux MF, O'Connell HE. Effect of length of liquid path on plate efficiency. *Chemical*
1325 *Engineering Progress*. 1955;51(5):232-237.
- 1326 65. Guinness R. Column performance in the rectification of petroleum. *Industrial and*
1327 *Engineering Chemistry*. 1937;29(10):1092-1100.
- 1328 66. Miyauchi T, Vermeulen T. Longitudinal dispersion in two-phase continuous-flow
1329 operations. *Industrial and Engineering Chemistry Fundamentals*. 1963;2(2):113-126.

- 1330 67. Bruin S, Freije AD. A simple liquid mixing model for distillation plates with stagnant
1331 zones. *Transactions of the Institution of Chemical Engineers*. 1974;52:75-79.
- 1332 68. Ashley MJ, Haselden GG. The calculation of plate efficiency under conditions of finite
1333 mixing in both phases in multiplate columns, and the potential advantage of parallel
1334 flow. *Chemical Engineering Science*. 1970;25(11):1665-1672.
- 1335 69. AIChE. *Bubble-tray Design Manual - Prediction of fractionation efficiency*. American
1336 Institute of Chemical Engineers; 1958.
- 1337 70. Molnar K. Eddy-diffusion coefficient in valve tray distillation columns. *Periodica*
1338 *Polytechnica Mechanical Engineering*. 1974;18(2-3):155-166.
- 1339 71. Barker PE, Self MF. The evaluation of liquid mixing effects on a sieve plate using
1340 unsteady and steady state tracer techniques. *Chemical Engineering Science*.
1341 1962;17(7):541-554.
- 1342 72. Bennett DL, Grimm HJ. Eddy diffusivity for distillation sieve trays. *AIChE Journal*.
1343 1991;37(4):589-596.
- 1344 73. Foss AS, Gerster JA, Pigford RL. Effect of liquid mixing on the performance of bubble
1345 trays. *AIChE Journal*. 1958;4(2):231-239.
- 1346 74. Gerster JA, Hill AB, Hochgraf NN, Robinson DG. *Tray Efficiencies in Distillation Columns-*
1347 *Final Report from the University of Delaware*. American Institute of Chemical
1348 Engineers;1958.
- 1349 75. Gilbert T. Liquid mixing on bubble-cap and sieve plates. *Chemical Engineering Science*.
1350 1959;10(4):243-253.
- 1351 76. Welch N, Durbin L, Holland C. Mixing on valve trays and in downcomers of a distillation
1352 column. *AIChE Journal*. 1964;10(3):373-379.
- 1353 77. Harada M, Adachi M, Eguchi W, Nagata S. Studies of fluid mixing on sieve plates.
1354 *International Chemical Engineering*. 1964;4(1):165.
- 1355 78. Sterbacek Z. Liquid dispersion coefficients on perforated plates with downcomers.
1356 *Transactions of the Institution of Chemical Engineers*. 1968;46(5):T167.

- 1357 79. Zuiderweg F. Sieve trays: a view on the state of the art. *Chemical Engineering Science*.
1358 1982;37(10):1441-1464.
- 1359 80. Zuiderweg F, de Groot J, Meeboer B, van der Meer D. Scaling up distillation plates. Paper
1360 presented at: Proceedings of the International Symposium on Distillation, England 1969.
- 1361 81. Wehner JF, Wilhelm RH. Boundary conditions of flow reactor. *Chemical Engineering*
1362 *Science*. 1956;6(2):89-93.
- 1363 82. Lim CT, Porter KE, Lockett MJ. The effect of liquid channelling on two-pass distillation
1364 plate efficiency. *Transactions of the Institution of Chemical Engineers*. 1974;52:193-201.
- 1365 83. Solari RB. *Liquid mixing and efficiency on non-ideal distillation trays* [Doctoral
1366 dissertation], University of California, Davis; 1974.
- 1367 84. Bell RL, Solari RB. Effect of nonuniform velocity fields and retrograde flow on distillation
1368 tray efficiency. *AIChE Journal*. 1974;20(4):688-695.
- 1369 85. Foss AS. *Liquid mixing on bubble trays and its effect upon plate efficiency* [Doctoral
1370 dissertation], University of Delaware; 1957.
- 1371 86. Stewart GN. Researches on the circulation time in organs and on the influences which
1372 affect it: Parts I—III. *The Journal of Physiology*. 1893;15(1-2):1.
- 1373 87. MacMullin RB, Weber M. The theory of short-circuiting in continuous-flow mixing
1374 vessels in series and the kinetics of chemical reactions in such systems. *Transactions of*
1375 *the American Institute of Chemical Engineers*. 1935;31(2):409-458.
- 1376 88. Andersen SL, Matthias RH. Prediction of catalyst activity in fluidized systems employing
1377 constant catalyst replacement rate. *Industrial and Engineering Chemistry*.
1378 1954;46(6):1296-1298.
- 1379 89. Danckwerts PV. Continuous flow systems: distribution of residence times. *Chemical*
1380 *Engineering Science*. 1953;2(1):1-13.
- 1381 90. Levenspiel O. *Chemical reaction engineering*. 3rd ed: John Wiley and Sons; 1999.
- 1382 91. Fogler HS, Gürmen MN. *Elements of chemical reaction engineering (online version)*. 4th
1383 ed: University of Michigan; 2008.

- 1384 92. Foss A, Gerster J. Liquid film efficiencies on sieve trays. *Chemical Engineering Progress*.
1385 1956;52(1):28.
- 1386 93. Paul EL, Atiemo-Obeng VA, Kresta SM. *Handbook of industrial mixing: science and*
1387 *practice*. John Wiley and Sons; 2004.
- 1388 94. Azizi F, Abou Hweij K. Liquid-phase axial dispersion of turbulent gas-liquid co-current
1389 flow through screen-type static mixers. *AIChE Journal*. 2017;63(4):1390-1403.
- 1390 95. Thakur R, Vial C, Nigam K, Nauman E, Djelveh G. Static mixers in the process industries—
1391 a review. *Chemical Engineering Research and Design*. 2003;81(7):787-826.
- 1392 96. Häfeli R, Hutter C, Damsohn M, Prasser H-M, von Rohr PR. Dispersion in fully developed
1393 flow through regular porous structures: experiments with wire-mesh sensors. *Chemical*
1394 *Engineering and Processing: Process Intensification*. 2013;69:104-111.
- 1395 97. Bennia A, Nahman N. Deconvolution of system impulse responses and time domain
1396 waveforms. *IEEE Transactions on Instrumentation and Measurement*. 1990;79:933-939.
- 1397 98. Bošković D, Loebbecke S. Modelling of the residence time distribution in micromixers.
1398 *Chemical Engineering Journal*. 2008;135:S138-S146.
- 1399 99. Essadki AH, Gourich B, Vial C, Delmas H. Residence time distribution measurements in an
1400 external-loop airlift reactor: Study of the hydrodynamics of the liquid circulation induced
1401 by the hydrogen bubbles. *Chemical Engineering Science*. 2011;66(14):3125-3132.
- 1402 100. Heibel AK, Lebens PJ, Middelhoff JW, Kapteijn F, Moulijn J. Liquid residence time
1403 distribution in the film flow monolith reactor. *AIChE journal*. 2005;51(1):122-133.
- 1404 101. Hutter C, Zenklusen A, Lang R, von Rohr PR. Axial dispersion in metal foams and
1405 streamwise-periodic porous media. *Chemical Engineering Science*. 2011;66(6):1132-
1406 1141.
- 1407 102. Mills P, Duduković M. Convolution and deconvolution of nonideal tracer response data
1408 with application to three-phase packed-beds. *Computers and Chemical Engineering*.
1409 1989;13(8):881-898.

- 1410 103. Mao Z-S, Xiong T, Chen J. Residence time distribution of liquid flow in a trickle bed
1411 evaluated using FFT deconvolution. *Chemical Engineering Communications*.
1412 1998;169(1):223-244.
- 1413 104. Parruck B, Riad SM. Study and performance evaluation of two iterative frequency-
1414 domain deconvolution techniques. *IEEE Transactions on Instrumentation and*
1415 *Measurement*. 1984;33(4):281-287.
- 1416 105. Pananakis D, Abel E. A comparison of methods for the deconvolution of isothermal DSC
1417 data. *Thermochimica Acta*. 1998;315(2):107-119.
- 1418 106. Saber M, Pham-Huu C, Edouard D. Axial dispersion based on the residence time
1419 distribution curves in a millireactor filled with β -SiC foam catalyst. *Industrial and*
1420 *Engineering Chemistry Research*. 2012;51(46):15011-15017.
- 1421 107. Gutierrez CG, Dias EF, Gut JA. Residence time distribution in holding tubes using
1422 generalized convection model and numerical convolution for non-ideal tracer detection.
1423 *Journal of Food Engineering*. 2010;98(2):248-256.
- 1424 108. Georget E, Sauvageat JL, Burbidge A, Mathys A. Residence time distributions in a modular
1425 micro reaction system. *Journal of Food Engineering*. 2013;116(4):910-919.
- 1426 109. Levenspiel O, Smith W. Notes on the diffusion-type model for the longitudinal mixing of
1427 fluids in flow. *Chemical Engineering Science*. 1957;6(4-5):227-235.
- 1428 110. Mohammed I, Bauer T, Schubert M, Lange R. Hydrodynamic multiplicity in a tubular
1429 reactor with solid foam packings. *Chemical Engineering Journal*. 2013;231:334-344.
- 1430 111. Dudukovic M, Felder R. Mixing effects in chemical reactors - IV - residence time
1431 distributions. *Reactor Stability, Sensitivity and Mixing Effects: AIChE Modular Instruction*
1432 *Series*; 1983:50-61.
- 1433 112. Sahai Y, Emi T. Melt flow characterization in continuous casting tundishes. *ISIJ*
1434 *international*. 1996;36(6):667-672.

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