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

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1	<u>Review Article</u>			
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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13 Abstract: Distillation columns are essential to chemical process industries, and most of them are fitted with cross-flow trays due to their versatility. Since these columns are expensive in terms 14 of cost and energy consumption, an accurate determination of their separation efficiency is a 15 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 particular, a comprehensive review of the existing theoretical efficiency prediction models along 23 with the critical analysis of their strengths and weaknesses is presented. The dependence of the 24

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

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

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35 **1. Background**

36 Distillation is the most important separation technology and will be pursued in the future simply due to the unavailability of industrially viable alternatives.¹ The physical separation of compo-37 38 nent substances from their mixture, called feed, is achieved in distillation columns.² Distillation columns are widely regarded as the workhorses of petroleum, chemical, petrochemical and re-39 lated process industries.³ These units consume approximately 3% of the total energy of the 40 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 equipments for improved designs as well as higher efficiencies. 46

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

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

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

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

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

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

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



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

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

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

 y_p and y_p^* are the vapor compositions that are actual and in equilibrium with the liquid at that point, respectively, as shown in Fig. 1. This definition of the vapor-side point efficiency is more realistic than the tray efficiency as it considers the composition variation along the tray.² The 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 profile.⁹ Analogous expressions for liquid-side tray and point efficiency can be formulated.^{2,3} The 88 tray efficiency is same as the point efficiency, when both liquid and vapor phases are completely 89 mixed. However, the Murphree tray efficiency is usually higher than the point efficiency due to 90 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 maximum mass transfer rate), which is same for both phases and lies within zero and unity. The 94 95 acknowledgement of any other efficiency concept than Murphree's by the process industry is yet to be noticed. Since the phases are partially mixed, a phenomenological model incorporating the 96 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



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Fig. 2. Classification of the tray efficiency.

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

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



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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 account for liquid maldistribution only. In general, the term 'flow non-idealities' is used to refer 117 to liquid maldistribution. On the contrary, no attempts to quantify the vapor non-idealities 118 through experiments have been made due to which the vapor flow is assumed in these models as 119 120 stated earlier. Besides, the plug flow of liquid is known to be beneficial for the efficiency and is termed 'ideal' for the trays. On the other hand, non-ideal flow patterns, such as liquid channeling, 121

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

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

Since the knowledge of the prevailing flow patterns is important for the evaluation of the tray efficiency, different experimental and numerical techniques have been devised to visualize the 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 In other studies, flow patterns were obtained from isotherms in the liquid, while the tray was 135 136 operated with hot water and cold air, and local liquid temperatures were measured with thermocouples¹⁰ and thermometers²³ at multiple locations. Multiple flow pointers, like weather 137 vanes, were also used to detect the flow direction on a tray, despite of being highly intrusive to 138 139 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 Bultitude²⁵ to obtain unidirectional velocity fields. However, the calibration of such probes is chal-142 143 lenging, as they need to be adjusted for every froth condition. Solari and Bell²⁶ and Bell^{27,28} extensively utilized fiber optic techniques and fluorescent tracer to acquire flow and mixing pat-144 terns using residence time profiles. Until now, the results from these experiments are preferably 145 used as validating criteria for numerical models (Computation Fluid Dynamics - CFD) discussed 146

later. Yu et al.²⁹ employed conductivity probes to trace the liquid flow using salt solution as tracer; however, the spatial resolution of recorded data is rather low. The nature of liquid flow at
different elevations above the tray deck was identified by Liu et al.³⁰ using a hot film anemometer. Recently, Schubert et al.¹⁸ used a wire-mesh sensor to measure the residence time distribution and velocity fields distributed on a tray at uniquely high spatial and temporal resolution. A
consolidated list of existing experimental techniques to identify the flow behavior on column
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 Ulbrich ¹⁰	Ø = 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 Bultitude ²⁵	Ø = 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 Kinnunen ²²	Ø = 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	Ø = 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	Ø = 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 Bell ²⁶	Ø = 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	Ø = 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	Ø = 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 re- circulation near the wall.
Liu et al. ³⁰	Ø = 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	Ø = 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**

In addition to the advances in experimental techniques, CFD has progressively emerged as an 157 important tool³⁰⁻⁴² for understanding the complex two-phase flows on distillation trays and to 158 forecast the tray performance at best prior to construction for various designs and operating 159 conditions.³⁴ In the past 25 years, several attempts have been made to model the tray hydrody-160 161 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. Interactions with the vapor phase were considered using interphase momentum transfer coeffi-164 165 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 the sieve tray hydrodynamics. They modeled the turbulent gas-liquid flow by assuming the mo-167 mentum exchange through bubble-liquid interactions only. It should be further mentioned that 168 their work was focused on small trays, where fluid dynamics is inconsistent with that of indus-169 170 trial trays. Also, they estimated the interphase momentum exchange coefficient based on the correlation of Bennett et al.⁴³, which overpredicts the liquid holdup fraction in the froth regime. 171 Liu et al.³⁰ studied the two-phase flow behavior on a sieve tray with a relatively simple two-172 173 dimensional model. They ignored the variations along the dispersion height in the direction of gas flow, modeled the gas action with an empirical equation and described the hydrodynamics of 174 the liquid phase only. Gesit et al.³⁴ employed a three-dimensional model and used the liquid 175 176 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 widely-varying predictions of the tray hydrodynamics.⁴⁵ Further, two-dimensional simulations 178 cannot account for the existing flow variations in the vertical dimension. Previously described 179 attempts were only concerned towards tray hydrodynamics, while they neglected mass and en-180 ergy conservation on sieve trays. As a result, Wang et al.³⁵ established a three-dimensional pseu-181 182 do-single-fluid model for obtaining liquid phase velocity and concentration distributions on

sieve trays in a 10-trayed column. A single-fluid model was preferred over a more accurate two-183 phase model for simulating an entire column due to its simplicity and low computational cost. 184 185 They performed the mass transfer studies for cyclohexane – n-heptane system and estimated the overall column efficiency using the Fenske-Underwood equation³⁵, which was overpredicted 186 with reference to Sakata and Yanagi⁴⁶. This method of determining the column efficiency using 187 end-product specifications is apt for approximate estimations only.⁴⁷ Error accumulation due to 188 189 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 this model. Rahimi et al.³⁶ and Noriler et al.^{37,38} extended the two-phase CFD model by consider-193 ing the energy and the chemical species conservation in a three-dimensional framework. They 194 195 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 and mass-transfer on sieve trays is questionable.⁴⁷ Zarei et al.⁴⁸ compared the hydrodynamic 198 performance of a mini V-grid (MVG) valve tray and a sieve tray with a two-phase three-199 dimensional model. The simulations indeed exhibited higher capacity for the MVG tray than for 200 201 the geometrically similar sieve tray, however, no experimental validation of the hydrodynamics of MVG valve tray was attempted in their work. The effect of the holes and bubble diameters on 202 hydraulics and mass transfer performance of two geometrically similar sieve trays was investi-203 gated by Rahimi et al.⁴⁹ using a three-dimensional two-phase model. They used a steady state 204 205 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 with a realizable $k - \varepsilon$ turbulence model to simulate the tray hydrodynamics on a cross-213 orthogonal fixed valve tray. Similar analysis was also done by Li et al.⁴¹ for a sieve tray with flow-214 guided holes and a bubble-promoter. The scope of their investigations were limited to hydrody-215 216 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 this model, thereby affecting the interface shape.⁵³ The prediction of clear liquid height through 220 221 this method was inconsistent with the Francis' equation and the experiment.⁴⁰ A hybrid approach of the volume of fluid (VOF) and a large eddy simulation (LES) model was developed by 222 223 Malvin et al.⁵⁴ to reduce the computational cost of the simulations. Although velocity predictions were in good agreement with Solari and Bell²⁶ experiments, the same is not true for the clear 224 liquid height with respect to Solari and Bell²⁶, Colwell⁴⁴ and Bennett et al.⁴³. Li et al.⁵⁵ proposed 225 226 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 performance with a conventional sieve tray, using two-phase three-dimensional model. Since no 228 229 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, using a VOF-like code with multiple size group (MUSIG) and shear stress transport (SST) model. 231 The total pressure drop of the ConCap tray was underpredicted by their model with respect to 232 their experiments⁵⁶. A consolidated summary of the reported CFD analyses of distillation trays is 233 234 given in Tab. 2.

Reference	Multiphase model	Tray setup; gas / liquid system	Observations
Mehta et al. ³¹	3D, steady state, single phase, contin- uum based model	Ø = 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,
Van Baten and Krishna ³³		\emptyset = 0.30 m sieve tray; water/air	liquid holdup distribution and clear liquid height
Liu et al. ³⁰	2D, steady state, single phase, k-ε 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 frac- tion profiles
Wang et al. ³⁵	3D, steady state, pseudo-single-phase, <i>k-ɛ</i> turbulence model	Ø = 1.22 m sieve trays (10 nos.) in a column; water/ air, and cyclohexane/ n-heptane	Liquid velocity distribution and vector plots, liquid concentration pro- files 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. Ø = 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	Ø = 0.35 m sieve tray; water/ air, and ethanol/ water	Liquid holdup, clear liquid height, pressure drop, gas and liquid veloci- ty profiles and streamlines, liquid velocity and temperature distribu- tions, mass and volume fraction, and point and tray efficiency
Zarei et al. ⁴⁸	3D, steady state, two phase, Euler-Euler	Ø = 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	Ø = 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	Ø = 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 <i>k-ɛ</i> model	Ø = 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	Ø = 1.21 m sieve tray; water/ air	Turbulent kinetic energy, clear liquid height, time-averaged liquid ve- locity 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 Ø = 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	Ø = 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

From the above model assessments, it can be easily observed that the majority of the hydrody-236 namic simulations are conducted for air-water system only, and validated with the experiments 237 238 of Solari and Bell²⁶. Even though large columns can have very different flow patterns than observed in the work of Solari and Bell²⁶. This is still considered as the state-of-the-art for CFD val-239 240 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. Velocity distribution and other hydraulic parameters should be used for this purpose to certify confi-242 243 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

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

regarding the measurement and simulations of flow non-uniformities. Instead, they simply as-262 263 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 uniform flow of homogenous vapor is only possible between small diameter trays.⁷ On large trays, 265 however, hydraulic gradients produce serious non-uniform vapor distributions.⁵⁷ Besides, few of 266 these models were formulated for rectangle-shaped trays.⁵⁸ The tray geometry, nevertheless, 267 268 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.

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

- were formulated for liquid dispersion in the flow direction only. This classification allows an
- easy interpretation of the model categories and is prepared out of authors' perception.



3. Modeling Methodologies of Separation Efficiency

294 The mathematical models are categorized hereinafter based on the flow and the mixing of liquid 295 on the tray. The first category comprises of the basic tray models that introduce the perfectly mixed and the plug flow of the liquid on a tray. The second category includes the pool models 296 that describe the liquid mixing through perfectly mixed stages in the flow direction. The diffu-297 sional models form the third category, where liquid mixing is considered via eddy diffusion 298 299 mechanism. The next category comprises of the non-uniform flow model that relates the nonideal flow profiles, in the absence of liquid mixing, with the tray efficiency. Lastly, the residence 300 time distribution (RTD) model describes the flow and the mixing patterns through liquid RTD 301

and evaluates their effect on the tray separation performance. Further description about thesemodels 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

$$E_{MV} = E_{OG} \quad . \tag{4}$$

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

314

315 3.1.2 Plug Flow Model

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

326

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

333 The models discussed so far demonstrate the two extremes of liquid mixing on a tray. As already334 stated, it is impossible to achieve the efficiency predicted by them due to incomplete or partial

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



341

342

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



343



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

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

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



354

355

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

356 The maldistribution factor, defined as

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

was devised to correlate the consequence of channeling with the tray separation performance. It
would be appropriate to call this factor as the coefficient of variation, as termed by Olujic' et al.⁶²
for the packed columns. In fact, this factor represents the normalized variation of the local liquid
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

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

377

378 3.2.1 Mixed Stages Model

Gautreaux and O'Connell⁶⁴ employed the Kirschbaum's idea of perfectly mixed stages on separation trays. They revisited the mixed pool concept and derived the equation

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

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





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

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

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

tween the axial dispersion model and the pool model assimilating backmixing amidst two consecutive pools.⁶⁷ The parameters for quantifying the liquid mixing are Péclet number (*Pe*) and number of pools in the dispersion model and the pool model, respectively. *Pe* and *n* denote continuous and discrete mixing in the respective methods. Further, Ashley and Haselden⁶⁸ confirmed that the axial dispersion and the pool model are equivalent for

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

and
$$Pe = 2n - 1$$
 for large Pe . (14)







403

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

404

405 3.2.2 Pool Cascade Model

Bruin and Freije⁶⁷ formulated a simple and versatile 'ready-to-use' model to incorporate the effects of channeling and stagnant regions on the tray efficiency. Here, the term versatility refers to the applicability of this method to a single-pass cross-flow tray of any design. This approach assumes the tray to be comprised of a cascade of identical mixing cells called main line mixers. 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.



416

415

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

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

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

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

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

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

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

Side mixer:
$$y'_{j} = mE_{OG}x'_{j} + (1 - E_{OG})y_{in}$$
 (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)

By solving Eqs. 15 to 18 recursively followed by using Eq. 19 and the assumption of linear vaporliquid 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)

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

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

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

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

Appendix A describes the mathematical treatment on Eq. 21 to obtain the preceding equation.
This was reported by Porter et al.²¹ as the limiting solution for large trays without any liquid
mixing. As far as the calculation of number of pools (Eq. 13) is concerned, it is advised to prefer
the definition given by AIChE's bubble tray design manual⁶⁹ as

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

448 This is the general definition of *Pe*, thus, it can be used for any tray design, and hence maintains the model's versatility. Here, τ is the mean residence time of the liquid whereas D_E is the eddy 449 450 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 to the tray design. An accurate determination of Pe or D_E is inevitable for unambiguous efficien-453 cy calculations. The readers are referred to these publications^{22,29,71-79} for further information on 454 455 the degree of liquid mixing on trays.

456 Experiments and simulations regarding the flow visualization on trays are essential to this model as they can provide the relative size of active and stagnant regions (i.e. ϕ_a and ϕ_d). To derive 457 458 β , the total exchanged flow between main line and side mixers is compared to the expected ex-459 change between active and stagnant regions by eddy diffusion.⁶⁷ Besides, the volatile material transport to the rising vapor in a semi-infinite stagnant region is considered,⁶⁷ due to which the 460 steady state penetration depth of the volatile component from active towards stagnant region is 461 equivalent to the 'width of mixing zone'.²¹ This comparison and the subsequent simplifications 462 yield 463

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

The term β_o is an empirical fitting parameter and can be treated like a constant. This parameter can be calculated by using the above equation in conjunction with Eq. 20 for a system with known efficiencies. Bruin and Freije⁶⁷ recommended this parameter to be 4 as a first approximation and validated the accuracy of this model through experimental data (Zuiderweg et al.⁸⁰ and Gerster et al.⁷⁴) and the eddy diffusion model²¹ (discussed in Section 3.3.2). The current model is in good agreement with the Porter's model²¹ but generally over-calculates the efficiencies by 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 stagnant regions ranging from 10% to 50% of the tray perforated area. These results are pre-472 sented using Eqs. 13 and 24 for the λE_{OG} values as 1 and 3. The prediction of the tray efficiency 473 474 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 efficiency loss is the highest for $\lambda E_{OG} = 3$. This inference is based upon the efficiency difference 477 between no stagnant region and largest stagnant region curves for the corresponding values of 478 479 *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 liquid mixing on the tray. Theoretically, high Péclet number corresponds to large-diameter trays 482 as well as lower liquid mixing on them, and vice-versa.²¹ Liquid mixing in the flow direction (i.e. 483 484 backmixing) is adverse to the tray efficiency, whereas transverse mixing is favourable for the tray performance.²⁰ Furthermore, λE_{OG} depends on the system and has an influence on the 485 cross-flow mixing on a tray.²¹ Higher liquid mixing orthogonal to the flow direction can be ex-486 pected for an increase in λE_{OG} . All these information may help in better interpretation of the 487 488 graphical results.



489



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) $\lambda E_{OG} = 3$.

In Fig. 12, a sharp rise in the tray efficiency for low values of the Péclet number is visible. This means that transverse mixing of the liquid is dominant at this instant, which equalizes any flow non-uniformity on the tray.²⁰ In other words, the cross-flow liquid mixing on small trays is strong enough to wipe out the stagnant regions. This rise in efficiency with respect to the Péclet number becomes gradual and continues until the mixing in flow direction is less significant as compared to the transverse mixing. A further increase in the Péclet number refers to relatively 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 situation becomes supportive for the formation of stagnant regions as the Péclet number further 503 504 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. Furthermore, Porter et al.²¹ emphasized the tendency of λE_{OG} to oppose the vapor bypassing. Thus, 507 an increase in cross-flow mixing and higher resistance to vapor bypassing can be expected at 508 509 higher λE_{OG} . These are the reasons behind improvement in the tray efficiency with increase in λE_{OG} . In addition, the position of the stagnant regions on large trays is also important. The ma-510 jority of the mass transfer on such trays happens in their first half, near the inlet downcomer.⁵⁸ 511 512 Therefore, the presence of any dead zone in the first half of a tray is highly disadvantageous for their separation performance. 513

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

The conclusive remarks about this model is that it is simple, versatile, ready-to-use and, is able to account for the effects of liquid channeling and stagnant regions on the tray efficiency. An improvement in this approach could be achieved by incorporating the effect of other nonuniformities in the liquid flow, such as retrograde flow and bypassing, as well as the location of dead zones on the tray fractionation performance. The determination of active and stagnant regions on a cross-flow tray, through simulations or experiments, has to be precise for this mod-

527 el to perform satisfactorily.



535 **3.3 Diffusional Models**

536 **3.3.1 AIChE Model**

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



544

545

Fig. 14. Schematic representation of the AIChE model.

Although the concept of eddy diffusion is explained for a rectangular bubble-cap tray, it is extendable to the trays of other design, too. Firstly, liquid and gas-phase transfer units are required to find the point efficiency. Subsequently, they are used in a mathematical model to predict the tray efficiency. Constant point efficiency and linear VLE curve are the assumptions in this model. Fig. 14 shows the liquid plug flow on the tray upon which the backmixing is superimposed through eddy diffusion. The model starts with the mass balance on the vertical slice of the aerated liquid on the tray, which results in

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

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

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

For convenience, the Péclet number in Eq. 23 is revised as $Pe = Z_1^2/(D_E \cdot \tau) = Z_1 \cdot (Z_1/\tau)/D_E = (Z_1V_f)/D_E$. This simplifies Eq. 26 as

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

558 The boundary conditions for the above equation are

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

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

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

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

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

Here, the tray efficiency depends on Pe and λE_{OG} only, out of which Pe requires an accurate determination of τ and D_E . As already mentioned in the pool cascade model, the eddy diffusion coefficient is influenced by the design of the tray.⁷⁰ The AIChE's report⁷⁴ gives a correlation of this coefficient for a rectangular bubble-cap tray; however, the flow patterns on circular trays can be very different than the idealized rectangular trays.²⁰ Further, the flow non-idealities are the characteristics of circular trays, except those of very small diameter.⁵⁸ Therefore, it is advised either to find the diffusion coefficient experimentally or to calculate it from correlations, for which the flow and the design parameters are within the range specified by the correlation. The efficiency predictions of this model have been validated for a 5.5 feet bubble-cap trayed column (methyl dichloride – ethylene dichloride system).⁶⁹ The AIChE model agrees well with the experimental efficiencies when they are below 100%, however, the predictions are overestimated, 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 the liquid mixing is significant on small trays, which eliminates the flow non-uniformities.²⁰ The 578 intensity of this efficiency rise, as mentioned in the Section 3.2.1, is proportional to λE_{OG} . Such 579 trend continues with increase in Péclet number until the liquid cross-mixing gets weaker and the 580 bulk liquid velocity becomes dominant for the material transfer.²⁰ This causes the efficiency to 581 582 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

high Pe, which is beyond the range of this figure. Since the cross-flow effect enhances with in-584 creasing λE_{0G} , it is straightforward to expect a higher efficiency for higher values of Pe and 585 λE_{OG} . However, large trays are susceptible to flow non-idealities, stagnant regions and eventual-586 ly vapor channeling due to which the efficiency should not rise but rather fall. Since this model is 587 designed to account for the liquid backmixing only, it is insensitive to non-uniform flow profiles 588 589 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 efficiency,^{21,58,67} which will be verified while comparing the results of the other models being 592 593 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-501 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

here due to symmetric concentration profiles on it.²⁶ An incremental area $(dz \cdot dw)$ over the tray
- having an aerated liquid (froth) with a uniform height h_f is considered. The transfer of mass into
- and out of this elemental froth is governed by the following mechanisms⁵⁸:
- (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.

$$(i) \left(L'_{z} + \frac{\partial L'_{z}}{\partial z} \frac{dz}{2}\right) \left(x + \frac{\partial x}{\partial z} \frac{dz}{2}\right) dw$$

$$(ii) \left(L'_{z} - \frac{\partial L'_{z}}{\partial z} \frac{dz}{2}\right) \left(x - \frac{\partial x}{\partial z} \frac{dz}{2}\right) dw$$

$$(iii) G' y_{in} dz dw$$

$$(iv) G' y(z,w) dz dw$$

$$(v) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} - \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

$$(vi) D_{E}h_{f}\rho_{L}\rho_{f} \left(\frac{\partial x}{\partial z} + \frac{\partial^{2} x}{\partial z^{2}} \frac{dz}{2}\right) dw$$

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

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

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

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

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

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

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

Eq. 33 is solved numerically with its associated boundary conditions using finite difference method. A detailed description on the finite-difference scheme, successive relaxation method and treatment of differentials near the wall are given in this publication.⁵⁸ Subsequently, the knowledge of the computed concentration profiles allows deriving the tray efficiency by following 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 and λE_{OG} . The flow of liquid is assumed to vary linearly in the *w*-direction. The ratio of the liquid 626 velocity at the wall and its mean value for any chord is denoted by q_s . Three values of q_s (0.5, 1.0 627 628 and 1.5) are considered to account for three different velocity profiles, as shown in Fig. 17. The stream functions corresponding to each profile have been calculated and supplied to Eq. 33. All 629 630 previously stated equations in this model were solved numerically and the efficiencies obtained for different values of Pe are shown in Fig. 17. It is straightforward that the efficiency is highest 631 during the chordal flow of liquid ($q_s = 1.0$). In addition, a uniform residence time distribution 632 exists on a tray at Pe = 200 and $q_s = 1$ due to which the efficiency approaches the solution of 633 Lewis' plug flow model.⁶⁰ This does not happen for the profiles corresponding to q_s values of 0.5 634 635 and 1.5.

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

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



646

Fig. 17. Tray efficiency for three different velocity profiles (dotted lines on the halved trays represent the stream function for the corresponding velocity profile).

Fig. 18 shows the performance of the eddy diffusion model for the tray with uniform (optimal) liquid flow i.e. $q_s = 1.0$. The tray efficiency follows the same trend as in Fig. 15 due to similar reasons stated in Section 3.3.1. The calculation of the concentration profiles on a tray corresponding to the liquid flow profile and subsequent determination of the tray efficiency demands plenty of computational effort. On the other hand, this remains the only model that considersliquid dispersion in the traverse as well as in the flow direction.





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 liquid mixing, on the tray efficiency.⁸⁴ The absence of liquid mixing is essential to sustain a veloc-660 661 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 alongside non-uniform velocity distributions. For simplicity, a rectangular tray was assumed to derive 664 the mathematical model. However, the model could be easily extended to circular tray geome-665 tries by increasing the flow path length near the wall.⁸⁴ No concentration gradients in the direc-666 tion normal to the main flow have been assumed. The coordinate system of this model is given in 667 Fig. 19a. 668





673Fig. 19. (a) Co-ordinate system with velocity distributions for the simple non-uniform flow674model for $q_s = 0$ and (b) schematics of the retrograde flow model.

Bell²⁸ and Solari⁸³ reported the general mass transport equation for a binary system, derived
from the species continuity equation, as

$$q \cdot \nabla x - \nabla \cdot \left(\dot{P}e^{-1} \right) \cdot \nabla x - \lambda E_{OG} \{ x_e^* - x(s,\xi) \} = 0 \quad . \tag{39}$$

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

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

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

$$\frac{E_{MV}}{E_{OG}} = \frac{\left[\int_{0}^{1} \frac{q(\xi)}{\lambda E_{OG}} \left\{1 - exp\left(-\frac{\lambda E_{OG}}{q(\xi)}\right)\right\} d\xi\right]}{\left[\int_{0}^{1} q(\xi) \left\{exp\left(-\frac{\lambda E_{OG}}{q(\xi)}\right)\right\} d\xi\right]}$$
(41)

Three velocity distributions, namely inverted parabolic, linear and parabolic (see Fig. 19a) are analyzed here. The inverted parabolic distribution corresponds to severe channeling along the tray centerline, while the parabolic distribution closely resembles the uniform flow. q_s is the normalized slip velocity at the wall and is considered zero in Fig. 19a for simplicity. It is also a 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. Due to resemblance with uniform flow, the parabolic distribution seems more advantageous for 691 692 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, i.e. parabolic velocity distribution. Hence, the difference in the separation performance of these 697 distributions is larger at higher values of λE_{OG} . 698

A peculiar observation about the inverted parabolic profile is that the E_{MV}/E_{OG} ratio at smaller 699 700 values of λE_{OG} is less than unity for this distribution with a zero slip velocity at the wall. Foss et al.⁷³ also proclaimed the drop of the tray efficiency below point efficiency that approaches zero 701 for bypassing liquid. This fact contradicts the possibility of the tray efficiency to fall between the 702 703 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

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. 19b. The forward and the retrograde flow regions are separated by a line, where the liquid ve-711 locity is zero. This type of model has been termed as the 'non-uniform retrograde flow model' 712 and is further classified into two sub-categories. In the first model, the liquid flowing through the 713 forward flow path is perfectly mixed at the outlet. A fraction of this uniform composition liquid 714 715 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 velocity line are directly rotated to the retrograde flow region and is therefore named as 'external rotation model'. This causes the liquid near the tray centerline in the forward flow region to flow near the wall in the retrograde flow region. Here, the liquid composition varies across the inlet of the retrograde zone opposite to the uniform composition model. The expression of the tray efficiency for these cases can be derived by following a similar procedure as employed in the simple non-uniform flow model.⁸⁴

723

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

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

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

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

- (i) liquid entering the tray consists of an infinite number of streams, each of which residesfor 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

43



744

Fig. 21. Schematic representation of the RTD model.

The concentration of the dissolved material in each stream is affected by the mass transfer to the 745 gas at local efficiency and by exchange with its local surroundings.⁸⁵ A froth element residing on 746 the tray for a time ranging between t and t + dt is subjected to the mass balancing. The total 747 material balance over the whole tray can be setup by summation over all fluid elements, if their 748 residence time distribution is known. Fig. 21 displays an aerated element with the cross-749 750 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

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

753 Similarly, the mean residence time of all streams is

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

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

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

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

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

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

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

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

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

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

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

The procedure to calculate the point efficiency is briefly introduced in the AIChE model in Section 3.3.1. If the point efficiency is supposed to be constant, then the tray efficiency can be expressed 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)

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

The dependency of the tray fractionation efficiency on f(t) and λE_{OG} is evident from Eq. 49. As 773 774 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 stimulusresponse experiments further enable to extract the flow patterns on the trays.^{18,26-28} The cor-779 780 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 efficiency (approximately 5%) due to non-uniform froth conditions at the liquid entrance.⁷³ 782

783 There is a severe lack of data concerning the residence time function of liquid on cross-flow trays. Foss et al.⁷³ conducted the tracer experiments on a rectangular sieve tray that was 36 784 785 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 functions with their mean residence time at different load conditions are exemplarily presented in 788 Fig. 22a.⁷³ The curve with the mean residence time of 15.7 s corresponds to liquid flow rate of 789 17.49 cm³/(cm·s) and gas flow rate of 1.84 m³/(m²·s). Similarly, the curve with the mean resi-790 791 dence time of 2.98 s corresponds to liquid and gas load of 90.04 $\text{cm}^3/(\text{cm}\cdot\text{s})$ and 1.83 $\text{m}^3/(\text{m}^2\cdot\text{s})$,

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



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

mean residence time at higher liquid flow rate and vice-versa at constant gas flow is obvious. 802 803 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 this, the position of the peak of these curves relative to their mean is very important for the di-805 806 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 computation is intended only for highlighting the effects of flow and mixing patterns via distribution 809 810 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.

A weak point of the RTD studies is that they are unable to uniquely determine the nature,⁹³ as 818 819 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 number of repetitions of the diffusive mechanism and, is incapable of handling extreme liquid 823 824 bypassing.⁷³ The RTD model, however, is capable of addressing these possibilities. The feasibility of tracer-response experiments further makes this model a prominent choice for the efficiency 825 826 predictions, especially in industry.

827

4. Comparison of Modeling Schemes

In order to compare the results of the existing models, the factors on which these models rely need to be considered. λE_{OG} and Pe appear in almost every model, while the other factors are weir length to diameter ratio,⁵⁸ relative size of active and stagnant regions,⁶⁷ liquid composition,⁵⁸ and residence time function.⁷³ This diversity in factors hinders the straightforward comparison of the models on a common ground. Thus, an attempt to collate the results from some of the existing methods at arbitrarily selected values of Pe for the usual range of λE_{OG} is demonstrated 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 AIChE model [3.3.1] at Pe = 50 practically coincide. These models consider the liquid backmix-838 839 ing only and are unconcerned towards the stagnant regions due to which the results from the pool cascade model [3.2.2] at $\beta_o = 4$ are also presented. It is obvious that the size of the stagnant 840 regions is proportional to the loss in the tray efficiency. The influence of λE_{OG} and Péclet number 841 on the tray efficiency has been discussed several times in this work. However, this model com-842 parison is only applicable for the tray assuming uniform liquid flow at the inlet. Apart from this, 843 844 Bell and Solari⁸⁴ reported that the tray efficiency becomes less than the point efficiency for an inverted parabolic velocity profile of liquid at the inlet (see Fig. 20). The pool cascade model also 845 provides similar observation (not shown here) e.g. the E_{MV}/E_{OG} ratio goes below unity for rela-846 847 tive stagnant regions larger than 80% at Pe = 5.



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Fig. 23. Comparison of efficiency predictions from different tray models at (a) Pe = 5 and (b) Pe = 50.

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

vapor distributions in the model formulation. Further, the 'Hybrid modeling' approach combin-859 860 ing experimentally validated CFD and tray efficiency models seems to be a promising alternative for realistic efficiency predictions. Such hybrid approach could be preferred in the future as 'vir-861 862 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 outlet, without giving any preference to the flow scenario at intermediate locations (except in 866 867 the eddy diffusion model). This is similar to the treatment of distillation trays as black box. Therefore, an account of the intermediate flow conditions in phenomenological models for 868 evolving tray efficiencies is another necessity. 869

Tab. 4: Summarization of existing tray models according to their respective account of flow patterns and liquid mixing on the tray. (\checkmark Acknowledged, \times Overlooked)

Model	Liquid mixing Flow direc- Transverse		Flow pat- terns	Remarks
	tion	direction		
3.1.1. Perfectly mixed model	V	/	x	Considers uniform liquid compo- sition over the tray
3.1.2. Plug flow model		×		Predicts the maximum achievable efficiency
3.1.3. Multi-channel plug flow model	X	¢	\checkmark	Accounts for liquid channeling only
3.2.1. Mixed stages model	\checkmark	×	x	Sensitive to backmixing of liquid only
3.2.2. Pool cascade model	\checkmark	\checkmark	x	Concerned towards channeling and stagnant zones
3.3.1. AIChE model	\checkmark	×	x	Most popular; accounts for liquid backmixing only
3.3.2. Eddy diffusion model	\checkmark	\checkmark	\checkmark	Most all-round model yet compu- tationally expensive
3.4. Non-uniform flow model	X	¢	\checkmark	Capable of distinguishing be- tween the effects of velocity pro- files on tray efficiency
3.5. RTD model	\checkmark	x	\checkmark	Most realistic model to account for flow patterns and liquid mix- ing in the flow direction

5. From Experiments to Efficiency Predictions: A Roadmap

One obvious question that remain unanswered is that how to utilize the experimental studies for 873 874 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 Solari and Bell²⁶ and Schubert et al.¹⁸, while using fibre-optic system and conductivity wire mesh 876 877 sensor (WMS) respectively. The latter study is favored for the aforementioned purpose due to the availability of data at comparatively high spatial and temporal resolution. In this investiga-878 879 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 on one of the trays. The effects of liquid load and outlet weir design on the flow patterns were 881 882 evaluated through the dispersion of salt (Na₂SO₄) 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 readers are referred to Schubert et al.¹⁸ for further details on column design, data calibration 885 886 and flow visualization.

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

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

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

convolution integral, whose calculation is straightforward.^{90,94} The converse of this integral is 896 897 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 WMS boundaries permit to use the Gaussian function for the open-open boundary 903 904 condition90,101,109 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)

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

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

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

$$R(t) = \frac{c(t)}{\int_0^\infty c(t)dt} \quad .$$
(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 sys925 tem⁹⁰ as

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

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

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

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

The estimation of the RTD enables computing the relative active and stagnant volumes on the tray. Duduković and Felder¹¹¹ suggested the tail of the impulse response function, accountable for the stagnant volume, to be truncated to acquire the active volume. Such truncation is researcher's perception dependent, and can lead to inconsistent fractions. Sahai and Emi¹¹² proposed that any fluid staying in a system for a period longer than twice the mean residence time can be considered as the stagnant or dead volume. Using this theory, the relative stagnant areadue 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 associated parameters as presented in Fig. 24. A good agreement between the convoluted func-940 941 tion and the WMS outlet response (shown for the lower liquid flow) is apparent in Fig. 24a. On comparison with higher liquid flow on the tray, lower liquid load exhibits higher residence time, 942 943 smaller Péclet number and larger percentage of liquid stagnancy, yet there is little difference in their numerical values (refer Fig. 24b). 944

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Fig. 24. (a) Response and convoluted function at the WMS boundaries for lower liquid flow and

(b) tray RTD functions with associated parameters.



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

The RTD model, the AIChE model and the pool cascade model are used to predict the tray effi-961 962 ciency for the assumed λE_{OG} . The mixed pool model is the limiting case of the pool cascade model for no stagnant liquid, while the eddy diffusion model requires serious computational effort 963 964 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 relatively higher for the higher liquid flow. This justifies that higher Péclet number and smaller 968

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

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979 6. Concluding Remarks and Perspective

Flow and mixing patterns on cross-flow trays are significant for their separation efficiency. The 980 981 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 mathematical models for calculating the tray efficiency. The development of new tray efficiency models or 984 985 improvements in the existing ones is desired parallel to advances in CFD modeling and measurements. In order to make these columns cost and energy efficient, an improvement in mass-986 transfer characteristics of column trays through design modification and revamping seems to be 987 988 a potential nomination. This is possible after their efficiency is accounted accurately. This serves as a motivation for further advancements in the efficiency modeling so that a better interpreta-989 990 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 validated CFD models, could be preferred in the future for tray efficiency predictions. Therefore, 992 the experimental and the simulation studies intended for column tray flow patterns have been 993 994 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 antici-999 pated 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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1008

1009 8. Nomenclature

1010	Α	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	<i>c</i> ₁ , <i>c</i> 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	Eo	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/(m²·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 ·s))
1030	L	Liquid flow rate (kmol/s)
1031	L'	Liquid flow rate per unit weir length (kmol/(m·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	'n	Dimensionless distance normal to the column wall (-)
1037	Ре	Péclet number (= $Z_1^2/(D_E \cdot \tau)$ (-)
1038	Р́е	Péclet number denoting the three-dimensional eddy mixing (-)
1039	р	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	<i>r</i> ₁ , <i>r</i> ₂	Roots of the differential equation in Appendix B (-)
1046	S	Non-dimensional distance in the flow direction from the inlet weir (-)

1047	Т	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	<i>w</i> ′	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	<i>x'</i>	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	<i>x</i> _m	Composition of liquid leaving the tray (-)
1062	<i>x</i> _{+<i>m</i>}	Liquid composition at the inlet weir (-)
1063	<i>x</i> _{<i>m</i>1}	Liquid composition at the inlet of the retrograde flow zone (-)
1064	<i>x</i> _{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	у	Composition (mole fraction) of the volatile component in the vapor phase (-)
1069	<i>y</i> ′	Composition (mole fraction) of the volatile component in the vapor phase in the
1070		side mixers (-)
1071	\mathcal{Y}_m	Composition of vapor leaving the tray (-)
1072	\mathcal{Y}_m^*	Composition of vapor in equilibrium with liquid leaving the tray (-)
1073	Yin	Composition of vapor entering the tray (-)

1074	\mathcal{Y}_p	Composition of vapor at point <i>p</i> on the tray (-)
1075	\mathcal{Y}_p^*	Composition of vapor in equilibrium with liquid at point p on the tray (-)
1076	\mathcal{Y}_2	Composition of vapor leaving the froth element in the AIChE model (-)
1077	Z_1	Flow path length (m)
1078	Ζ	Distance from inlet weir in the flow direction (m)
1079	<i>z'</i>	Normalized distance from inlet weir in the flow direction (= z/D) (-)
1080		
1081	Subscripts	
1082	а	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	т	<i>mth</i> tray
1092	mean	Mean or average
1093	W	w - direction
1094	Ζ	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 direc-
1107		tion (-)
1108	$ ho_L$	Clear liquid density (kmol/m ³)
1109	$ ho_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	$ au_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	Abbreviatio	ns

- 1120AIChEAmerican Institute of Chemical Engineers
- 1121*CFD*Computational fluid dynamics
- **1122***LES*Large eddy simulation

1123	MDF	Maldistribution factor
1124	RTD	Residence time distribution
1125	SA	Stagnant area
1126	VLE	Vapor-liquid equilibrium
1127	VOF	Volume of fluid
1128	WMS	Wire mesh sensor
1129	2 <i>D</i>	Two-dimensional
1130	3 <i>D</i>	Three-dimensional
1131		

1132 Appendix (A)

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

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

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

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

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

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

1136 Using the binomial expansion, one can write

$$\left(1+\frac{1}{U}\right)^{U} = {}^{U}C_{0} \cdot 1^{U} \cdot (1/U)^{0} + {}^{U}C_{1} \cdot 1^{U-1} \cdot (1/U)^{1} + {}^{U}C_{2} \cdot 1^{U-2} \cdot (1/U)^{2} + \cdots$$
$$= 1+1+\frac{U-1}{2U} + \frac{(U-1)(U-2)}{6U^{2}} + \cdots = 1+1+\frac{1}{2} - \frac{1}{2U} + \frac{(1-1/U)(1-2/U)}{6} + \cdots$$
(A3)

1137 The application of the limit in Eq. A3 provides

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

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

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

1139

1140 Appendix (B)

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

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

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

$$X'' - Pe X' - \lambda E_{0G} Pe X = 0 \quad . \tag{B1}$$

1143 The solution of Eq. B1 is given by

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

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

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

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

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

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

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

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

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

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

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

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

1151

1152 Appendix (C)

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

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

1154 The equation of continuity is

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

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

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

$$L'_{z} = h_{f} \rho_{L} \rho_{f} \frac{\partial \psi}{\partial w} \quad , \tag{C3}$$

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

$$L = 2h_f \rho_L \rho_f \psi_o \quad , \tag{C5}$$

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

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

$$Pe = \frac{DL}{h_f \rho_L \rho_f W D_E} \quad . \tag{C7}$$

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

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

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

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

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

1164

1165 Appendix (D)

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

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

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

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

$$\int_{0}^{\infty} f(t) \left[\frac{dx(s,t)}{ds} + \lambda E_{OG} \frac{t}{\tau} \{ x(s,t) - x_{e}^{*} \} + \frac{KAZ_{1}}{L} \frac{t}{\tau} \left\{ x(s,t) - \int_{0}^{\infty} x(s,t) \frac{t}{\tau} f(t) dt \right\} \right] dt = 0 \quad (D2)$$

1170 The mean residence time is defined as

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

1171 Using Eq. D3, Eq. D2 transforms to

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

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

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

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

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

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

1175 The Murphree efficiency for the liquid-side is

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

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

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

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



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

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

1183

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