

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

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1 **Review Article**

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

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

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

31

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

34

## 35 **1. Background**

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

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

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

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

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

61 This is also known as the overall stage efficiency. Here,  $N_{eq}$  is the number of equilibrium stages,  
62 obtained from equilibrium design calculations (McCabe-Thiele method), the Fenske-  
63 Underwood-Gilliland method, process engineering softwares or from others,<sup>2</sup> while  $N_{ac}$  is the  
64 actual number of trays in a column. The achievement of separation on a cross-flow tray is usual-  
65 ly described by the (Murphree<sup>6</sup>) tray efficiency. It is the ratio of the actual change in vapor<sup>1</sup> com-  
66 position on a tray over its composition change for an equivalent equilibrium stage, according to

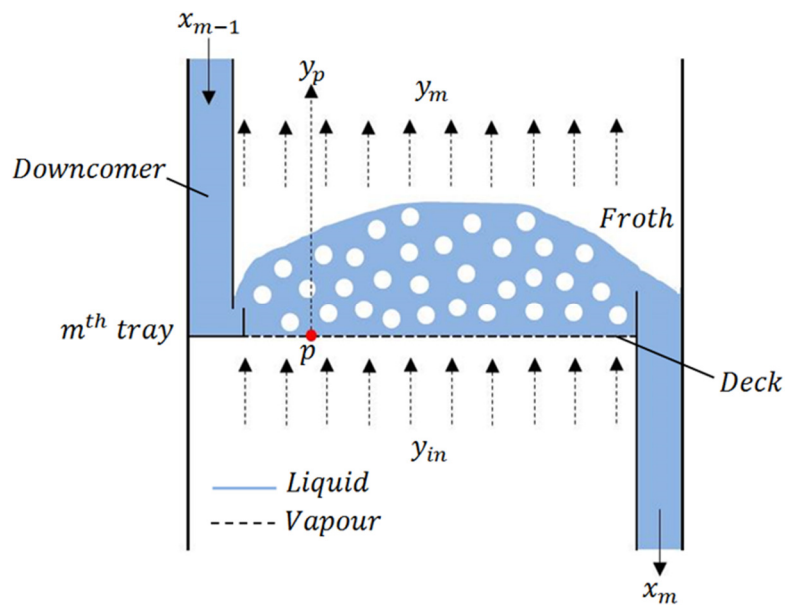
$$E_{MV} = \frac{y_m - y_{in}}{y_m^* - y_{in}} \quad . \quad (2)$$

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

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<sup>1</sup> The term 'gas' and 'vapor' are used interchangeably in this work.

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



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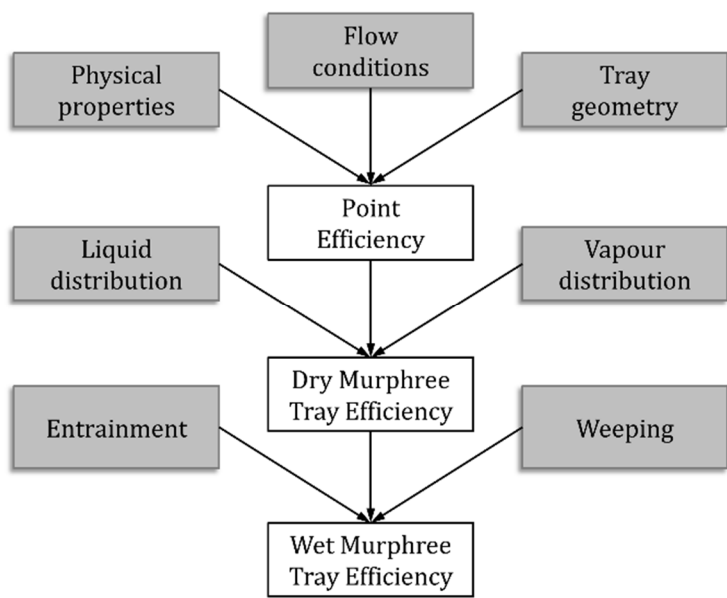
**Fig. 1.** Illustration for vapor-side tray and point efficiency.

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

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

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

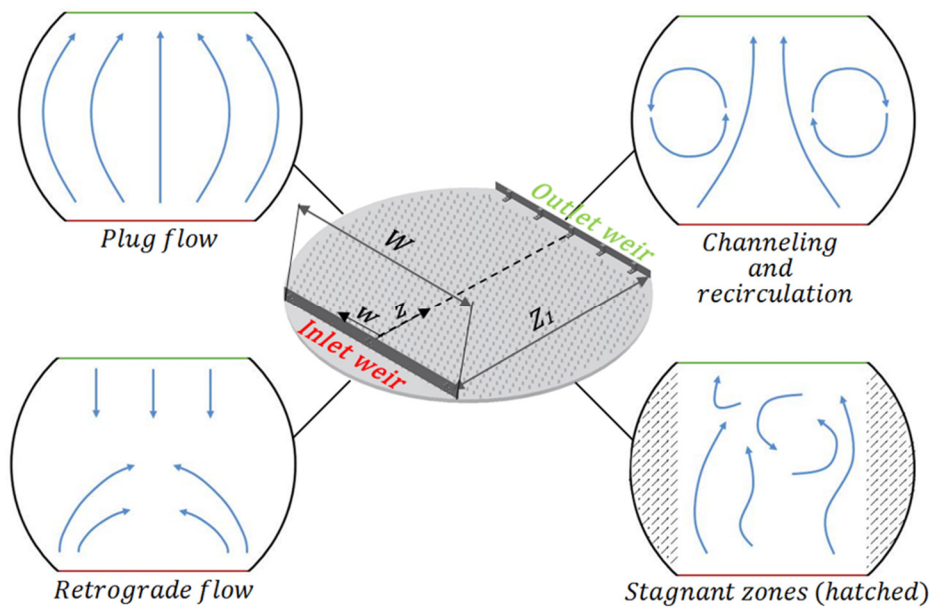
87 tion in the equilibrium vapor composition across the tray according to the liquid composition  
 88 profile.<sup>9</sup> Analogous expressions for liquid-side tray and point efficiency can be formulated.<sup>2,3</sup> The  
 89 tray efficiency is same as the point efficiency, when both liquid and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



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

103 Further classification of the tray efficiency and the factors affecting it can be understood from  
 104 Fig. 2.<sup>17</sup> The point efficiency refers to the mass transfer at a certain point on the tray depending

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



112

113

**Fig. 3.** Liquid flow patterns on a tray.

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

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

124

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

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

129

### 130 **2.1 Experimental Studies**

131 The simplest experimental method involved the usage of floats, such as table-tennis or cork  
132 balls, to pursue the flow of liquid.<sup>21,22</sup> 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.<sup>21</sup>  
135 In other studies, flow patterns were obtained from isotherms in the liquid, while the tray was  
136 operated with hot water and cold air, and local liquid temperatures were measured with ther-  
137 mocouples<sup>10</sup> and thermometers<sup>23</sup> at multiple locations. Multiple flow pointers, like weather  
138 vanes, were also used to detect the flow direction on a tray, despite of being highly intrusive to  
139 the flow itself.<sup>23</sup> Yet, infrared camera technique was used to visualize the fronts of inflowing hot  
140 liquid mixing with cold liquid.<sup>24</sup> The extraction of quantitative flow parameters with these tech-  
141 niques was still difficult. The strain gauge probe technique was employed by Biddulph and Bulti-  
142 tude<sup>25</sup> to obtain unidirectional velocity fields. However, the calibration of such probes is chal-  
143 lenging, as they need to be adjusted for every froth condition. Solari and Bell<sup>26</sup> and Bell<sup>27,28</sup> ex-  
144 tensively utilized fiber optic techniques and fluorescent tracer to acquire flow and mixing pat-  
145 terns using residence time profiles. Until now, the results from these experiments are preferably  
146 used as validating criteria for numerical models (Computation Fluid Dynamics - CFD) discussed



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

154

**Space left for Table 1**

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

Reference	Tray setup; gas/ liquid system	Technique	Observations
<b>Stichlmair and Ulbrich<sup>10</sup></b>	$\emptyset = 2.30$ m bubble-cap and sieve tray; hot water/ air	Thermocouples	Liquid isotherms indicate the extent of channeling; influence of modified inlet and outlet weirs, tray tilting and baffles on flow patterns.
<b>Biddulph and Bultitude<sup>25</sup></b>	$\emptyset = 0.69$ m sieve tray; water/ air	Strain gauge probe network	Axial velocity profiles show non-uniform flow of liquid with low velocities near the wall.
<b>Sohlo and Kinnunen<sup>22</sup></b>	$\emptyset = 0.50$ m sieve tray; water/ air	Floating cork balls	Non-ideal velocity profiles at low liquid flow rates and at high weir heights; plug flow behavior at high liquid flow rates and at low weir heights.
<b>Porter et al.<sup>23</sup></b>	$\emptyset = 2.44$ m sieve tray; hot water/ air	Thermometers, flow pointers	Substantial liquid recirculation at high weir loads and at low gas loads.
<b>Porter et al.<sup>21</sup></b>	$\emptyset = 1.20$ m sieve tray; water/ air	Photographic camera, dye injection, table-tennis balls	Existence of stagnant regions near the wall; tray tilting modifies the liquid flow patterns.
<b>Solari and Bell<sup>26</sup></b>	$\emptyset = 1.20$ m sieve tray; water/ air	Fiber-optic detection system, dye injection	Liquid pooling near the wall at low liquid and gas loads; effect of flow rates on this pooling; existence of non-ideal flow and mixing patterns.
<b>Li et al.<sup>24</sup></b>	$\emptyset = 1.20$ m sieve tray; water/ air	Thermal infrared camera, hot water injection	Flow non-uniformity on the tray with one downcomer; stagnant regions on multiple downcomer tray depicted through frontier curves.
<b>Yu et al.<sup>29</sup></b>	$\emptyset = 2.00$ m sieve tray; water/ air	Electrical conductivity probes, tracer injection	Non-uniform (parabolic) flow in the central part of the tray with slow recirculation near the wall.
<b>Liu et al.<sup>30</sup></b>	$\emptyset = 1.20$ m sieve tray; water/ air	Hot film anemometer	3D flow of liquid up to 10 mm above the tray deck and the flow becomes 2D beyond the aforementioned distance.
<b>Schubert et al.<sup>18</sup></b>	$\emptyset = 0.80$ m sieve tray; water/ air	Wire mesh sensor, tracer injection	Influence of liquid load and outlet weir on flow patterns; liquid RTD and weir-to-weir velocities portraying flow non-idealities.

## 156 2.2 CFD Simulations

157 In addition to the advances in experimental techniques, CFD has progressively emerged as an  
158 important tool<sup>30-42</sup> for understanding the complex two-phase flows on distillation trays and to  
159 forecast the tray performance at best prior to construction for various designs and operating  
160 conditions.<sup>34</sup> In the past 25 years, several attempts have been made to model the tray hydrody-  
161 namics. All CFD studies discussed here use the Eulerian framework, if not otherwise specified.  
162 Mehta et al.<sup>31</sup> predicted the steady-state three-dimensional flow of the liquid on a sieve tray,  
163 using time- and volume-averaged continuity and momentum equations for the liquid phase only.  
164 Interactions with the vapor phase were considered using interphase momentum transfer coeffi-  
165 cients determined from empirical correlations. Krishna et al.<sup>32</sup> and Van Baten and Krishna<sup>33</sup> ad-  
166 vanced the previous approach by proposing a three-dimensional two-phase model to simulate  
167 the sieve tray hydrodynamics. They modeled the turbulent gas-liquid flow by assuming the mo-  
168 mentum exchange through bubble-liquid interactions only. It should be further mentioned that  
169 their work was focused on small trays, where fluid dynamics is inconsistent with that of indus-  
170 trial trays. Also, they estimated the interphase momentum exchange coefficient based on the  
171 correlation of Bennett et al.<sup>43</sup>, which overpredicts the liquid holdup fraction in the froth regime.  
172 Liu et al.<sup>30</sup> studied the two-phase flow behavior on a sieve tray with a relatively simple two-  
173 dimensional model. They ignored the variations along the dispersion height in the direction of  
174 gas flow, modeled the gas action with an empirical equation and described the hydrodynamics of  
175 the liquid phase only. Gesit et al.<sup>34</sup> employed a three-dimensional model and used the liquid  
176 holdup correlation suggested by Colwell<sup>44</sup> to predict the flow patterns and hydraulics of a com-  
177 mercial-scale sieve tray. According to Kister<sup>3</sup>, different correlations can lead to inconsistent and  
178 widely-varying predictions of the tray hydrodynamics.<sup>45</sup> Further, two-dimensional simulations  
179 cannot account for the existing flow variations in the vertical dimension. Previously described  
180 attempts were only concerned towards tray hydrodynamics, while they neglected mass and en-  
181 ergy conservation on sieve trays. As a result, Wang et al.<sup>35</sup> established a three-dimensional pseu-  
182 do-single-fluid model for obtaining liquid phase velocity and concentration distributions on

183 sieve trays in a 10-trayed column. A single-fluid model was preferred over a more accurate two-  
184 phase model for simulating an entire column due to its simplicity and low computational cost.  
185 They performed the mass transfer studies for cyclohexane – n-heptane system and estimated the  
186 overall column efficiency using the Fenske-Underwood equation<sup>35</sup>, which was overpredicted  
187 with reference to Sakata and Yanagi<sup>46</sup>. This method of determining the column efficiency using  
188 end-product specifications is apt for approximate estimations only.<sup>47</sup> Error accumulation due to  
189 simultaneous solution of momentum and mass-transfer equation and the usage of eddy-  
190 diffusion coefficient from the correlations applicable for air-water system only are the other  
191 reasons behind this overprediction. The assumption of constant values for vapor (and liquid)  
192 volume fractions and the inability to predict point and tray efficiencies are further limitations of  
193 this model. Rahimi et al.<sup>36</sup> and Noriler et al.<sup>37,38</sup> extended the two-phase CFD model by consider-  
194 ing the energy and the chemical species conservation in a three-dimensional framework. They  
195 used correlations for momentum, heat and mass-transfer coefficients to predict hydrodynamics  
196 along with temperature and concentration distributions on rectangular and circular sieve trays.  
197 However, the employment of standard correlations and empirical models for simulating the heat  
198 and mass-transfer on sieve trays is questionable.<sup>47</sup> Zarei et al.<sup>48</sup> compared the hydrodynamic  
199 performance of a mini V-grid (MVG) valve tray and a sieve tray with a two-phase three-  
200 dimensional model. The simulations indeed exhibited higher capacity for the MVG tray than for  
201 the geometrically similar sieve tray, however, no experimental validation of the hydrodynamics  
202 of MVG valve tray was attempted in their work. The effect of the holes and bubble diameters on  
203 hydraulics and mass transfer performance of two geometrically similar sieve trays was investi-  
204 gated by Rahimi et al.<sup>49</sup> using a three-dimensional two-phase model. They used a steady state  
205 model, which is insufficient for modeling the dynamical behavior of distillation trays. Recently,  
206 several investigators focused on the application of CFD studies to non-conventional trays. Jiang  
207 et al.<sup>50</sup> and Li et al.<sup>39</sup> 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.<sup>51</sup> 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.<sup>52</sup> used a three-dimensional two-phase model  
213 with a realizable  $k-\epsilon$  turbulence model to simulate the tray hydrodynamics on a cross-  
214 orthogonal fixed valve tray. Similar analysis was also done by Li et al.<sup>41</sup> for a sieve tray with flow-  
215 guided holes and a bubble-promoter. The scope of their investigations were limited to hydrody-  
216 namics, while their predictions were inconsistent with the correlations and experimental  
217 data.<sup>41,52</sup> 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.<sup>40</sup> using the volume of fluid (VOF)  
219 method. The interface curvature and surface tension forces are difficult to model correctly with  
220 this model, thereby affecting the interface shape.<sup>53</sup> The prediction of clear liquid height through  
221 this method was inconsistent with the Francis' equation and the experiment.<sup>40</sup> A hybrid ap-  
222 proach of the volume of fluid (VOF) and a large eddy simulation (LES) model was developed by  
223 Malvin et al.<sup>54</sup> to reduce the computational cost of the simulations. Although velocity predictions  
224 were in good agreement with Solari and Bell<sup>26</sup> experiments, the same is not true for the clear  
225 liquid height with respect to Solari and Bell<sup>26</sup>, Colwell<sup>44</sup> and Bennett et al.<sup>43</sup>. Li et al.<sup>55</sup> proposed  
226 the concept of an 's' shaped distillation column fitted with elliptical sieve trays. They established  
227 the importance of this unconventional tray by comparing its hydraulics, RTD and mass-transfer  
228 performance with a conventional sieve tray, using two-phase three-dimensional model. Since no  
229 such column exists in reality, this study lacked the experimental validation of the predictions.  
230 Another unconventional tray known as conical cap (ConCap) tray was examined by Zarei et al.<sup>42</sup>,  
231 using a VOF-like code with multiple size group (MUSIG) and shear stress transport (SST) model.  
232 The total pressure drop of the ConCap tray was underpredicted by their model with respect to  
233 their experiments<sup>56</sup>. A consolidated summary of the reported CFD analyses of distillation trays is  
234 given in Tab. 2.

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

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

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

236 From the above model assessments, it can be easily observed that the majority of the hydrody-  
237 namic simulations are conducted for air-water system only, and validated with the experiments  
238 of Solari and Bell<sup>26</sup>. Even though large columns can have very different flow patterns than ob-  
239 served in the work of Solari and Bell<sup>26</sup>. This is still considered as the state-of-the-art for CFD val-  
240 idation irrespective of the recent experimental advances as mentioned in Tab 1. In addition, the  
241 clear liquid height is considered as the sole criterion for the validation of the CFD studies. Veloci-  
242 ty distribution and other hydraulic parameters should be used for this purpose to certify confi-  
243 dence on the simulations. According to Schultes<sup>45</sup>, 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.<sup>45</sup> 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.<sup>47</sup>

251

### 252 **2.3 Objective Viewpoints**

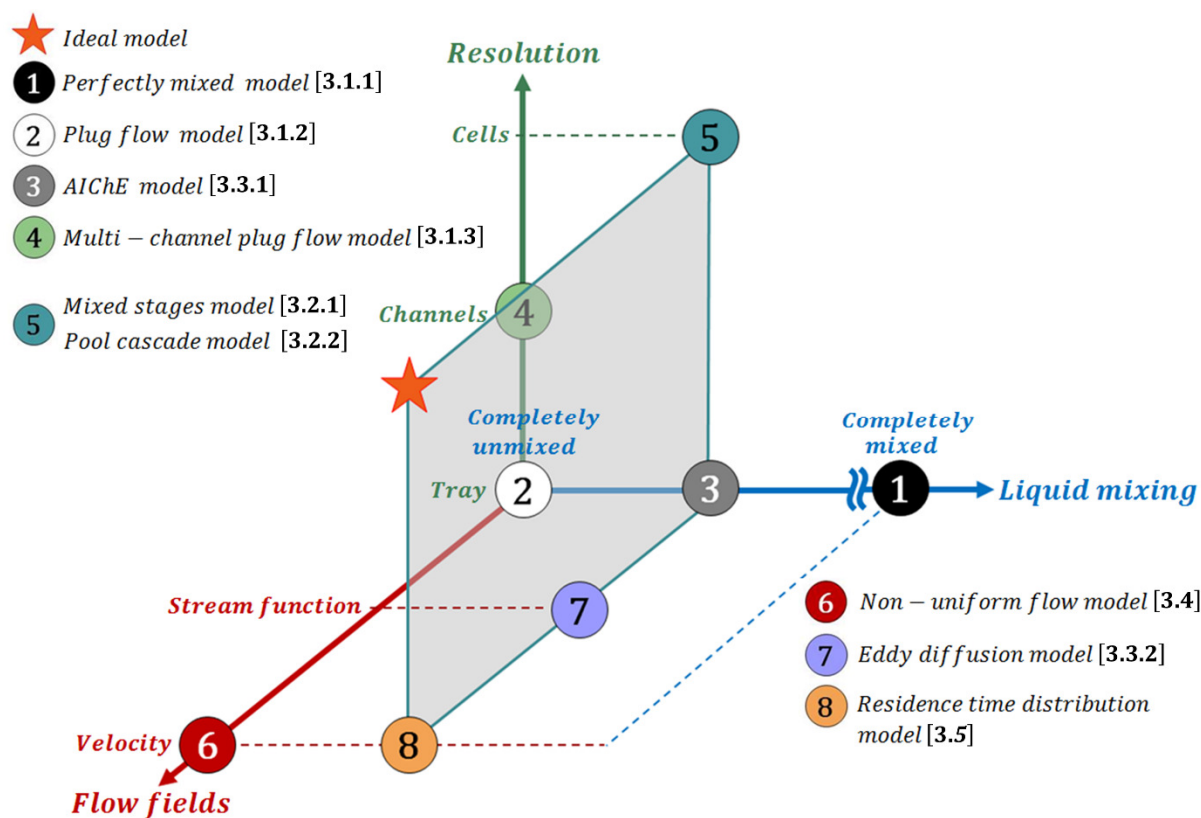
253 Despite of the concerns regarding mass transfer predictions, it is clear that CFD will be the part  
254 of the distillation modeler's toolbox in the near future to acquire the fluid dynamics on the trays.  
255 Therefore, a hybrid strategy is expected in the future considering CFD simulations to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



262 regarding the measurement and simulations of flow non-uniformities. Instead, they simply as-  
263 sume uniform liquid flow superimposed with mixing mechanism, uniform vapor flow with com-  
264 plete mixing between the trays, linear equilibrium curve and so forth. As stated earlier, the uni-  
265 form flow of homogenous vapor is only possible between small diameter trays.<sup>7</sup> On large trays,  
266 however, hydraulic gradients produce serious non-uniform vapor distributions.<sup>57</sup> Besides, few of  
267 these models were formulated for rectangle-shaped trays.<sup>58</sup> The tray geometry, nevertheless,  
268 plays a big role in shaping the flow on trays. The curved walls near the downcomer create the  
269 tendency of directing liquid towards the tray centerline. This channeling causes the flow to sepa-  
270 rate under certain conditions, thus, creating re-circulatory patterns.<sup>28</sup> In addition, Lockett and  
271 Safekourdi<sup>20</sup> 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, Taylor<sup>47</sup> also emphasized the need for understanding the formulation and solution of  
277 the model equations.

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

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



290

291

Fig. 4. Classification of tray efficiency prediction models.

292

### 293 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  
 296 mixed and the plug flow of the liquid on a tray. The second category includes the pool models  
 297 that describe the liquid mixing through perfectly mixed stages in the flow direction. The diffu-  
 298 sional models form the third category, where liquid mixing is considered via eddy diffusion  
 299 mechanism. The next category comprises of the non-uniform flow model that relates the non-  
 300 ideal flow profiles, in the absence of liquid mixing, with the tray efficiency. Lastly, the residence  
 301 time distribution (RTD) model describes the flow and the mixing patterns through liquid RTD

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

304

### 305 **3.1 Basic Tray Models**

#### 306 **3.1.1 Perfectly Mixed Model**

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

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

311 However, in 1934, Kirschbaum<sup>59</sup> observed gradients in the liquid composition on a small tray  
312 (only few inches in diameter) at high superficial gas velocities. These findings led to the devel-  
313 opment of tray models enlisted below.

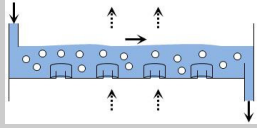
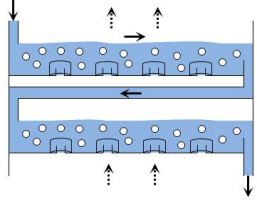
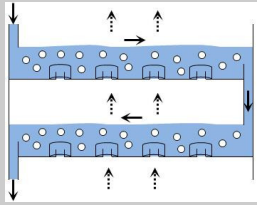
314

#### 315 **3.1.2 Plug Flow Model**

316 Lewis<sup>60</sup> firstly introduced the concept of plug flow on distillation trays. In this model, liquid is  
317 assumed to travel across a rectangular bubble-cap tray without being mixed in the flow direc-  
318 tion; however, there may be transverse mixing to any extent. The other assumptions are uniform  
319 liquid and vapor loads, linear vapor-liquid equilibrium curve and constant point efficiency  
320 throughout the tray. The material balancing over the tray yields the mathematical equations to  
321 predict the tray efficiency given in Tab. 3 for three different cases according to the liquid flow  
322 direction. These are the maximum achievable tray efficiencies for each case<sup>3</sup>. The efficiencies, in

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

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

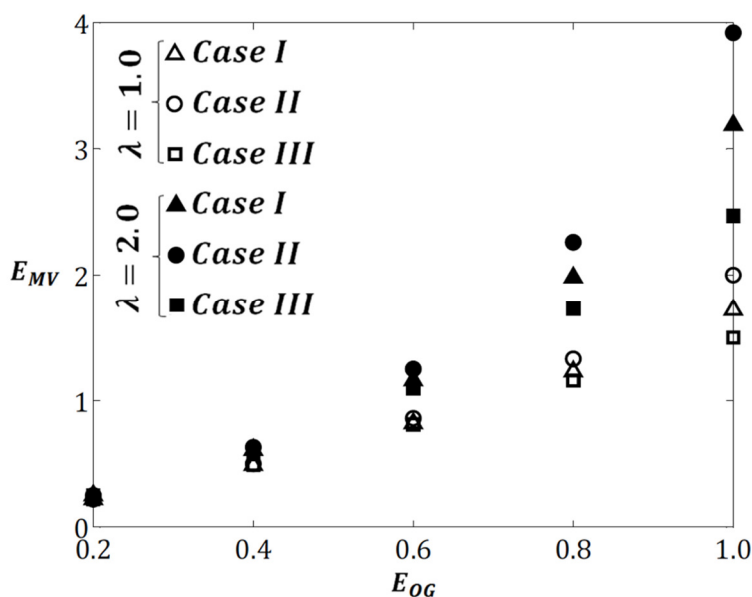
Cases	Description	Model
(I) Vapor entering the tray is completely mixed.		$E_{MV} = \{exp(\lambda E_{OG}) - 1\}/\lambda \quad (5)$ <p><math>\lambda</math> is called stripping factor and is defined as</p> $\lambda = b \cdot G/L. \quad (6)$
(II) Unmixed vapor rises upwards, while liquid flows in the same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

326

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

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

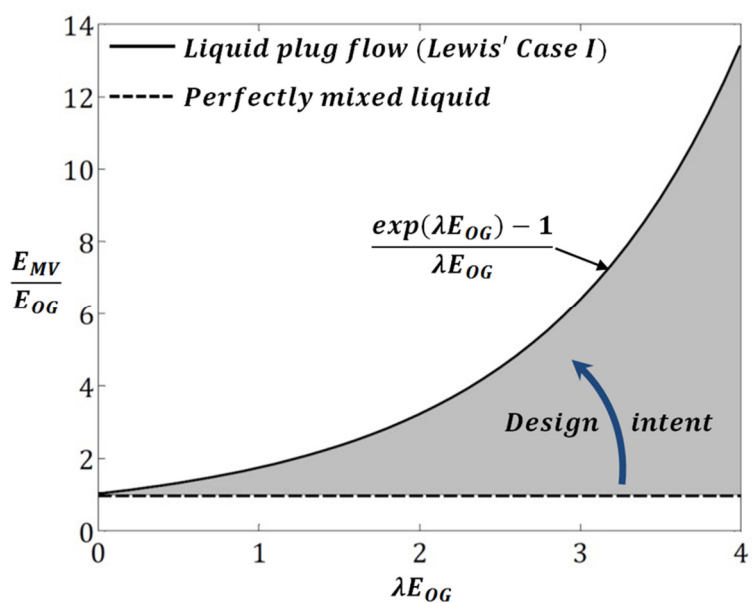
335 mixing of the liquid in reality. However, they provide an encapsulation of the separation efficien-  
 336 cy, presented as a grey shaded area in Fig. 6, within which the efficiency of a tray with real flow  
 337 and mixing conditions should always be.<sup>61</sup> Strictly speaking, this holds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



341

342

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



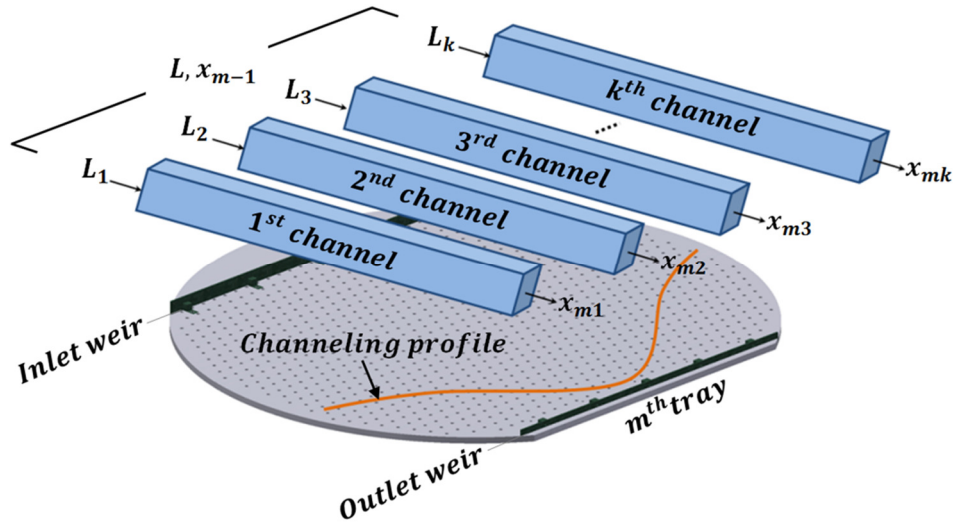
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344

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

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

346 Stichlmair and Ulbrich<sup>10</sup> observed channeling through distribution of liquid isotherms on bub-  
 347 ble-cap and sieve trays. To account for liquid channeling in this model, the tray is assumed to  
 348 consist of a large number of parallel channels, as depicted in Fig. 7. Plug flow behavior is as-  
 349 sumed in each channel with different flow rates in accordance with the channeling profile. This  
 350 assumption allows employing the Lewis' Case I to calculate the Murphree efficiency for each  
 351 channel. This efficiency and the mass balance permit to find the liquid composition exiting each  
 352 channel, for a given inlet composition. The averaging of the liquid composition from all channels  
 353 enables to compute the tray efficiency.



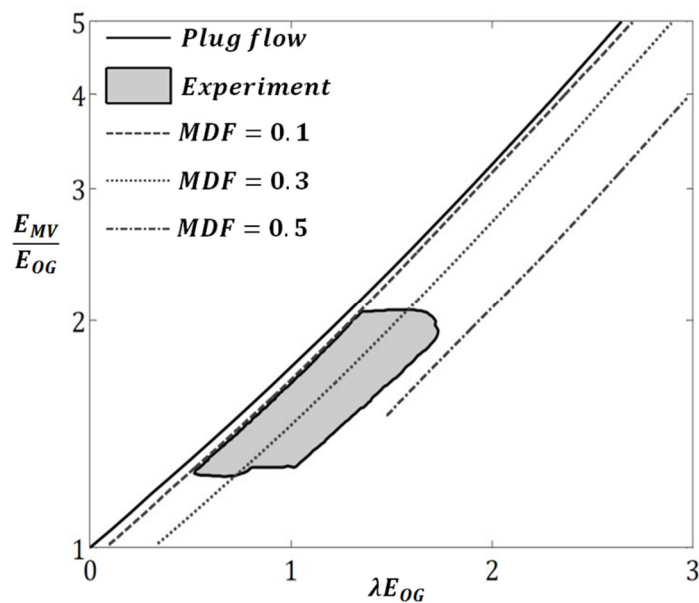
354  
 355 **Fig. 7.** Stichlmair's multi-channel plug flow model.

356 The maldistribution factor, defined as

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

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

361 mental data, obtained by Stichlmair and Ulbrich<sup>10</sup>, 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.<sup>10</sup> 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.

368

369

### 370 3.2 Liquid Pool Models

371 Kirschbaum<sup>63</sup> firstly proposed a model that considers the tray consisting of several identical  
 372 pools of completely mixed liquid. These pools account for liquid concentration gradients in the  
 373 flow direction. The liquid is assumed to flow through the pools one-by-one from inlet to outlet  
 374 weir. A tray with one pool and with an infinite number of pools can easily explain the limiting  
 375 cases of perfectly mixed and unmixed liquid, respectively. An intermediate number of pools cor-  
 376 respond to incomplete or partial mixing of liquid.

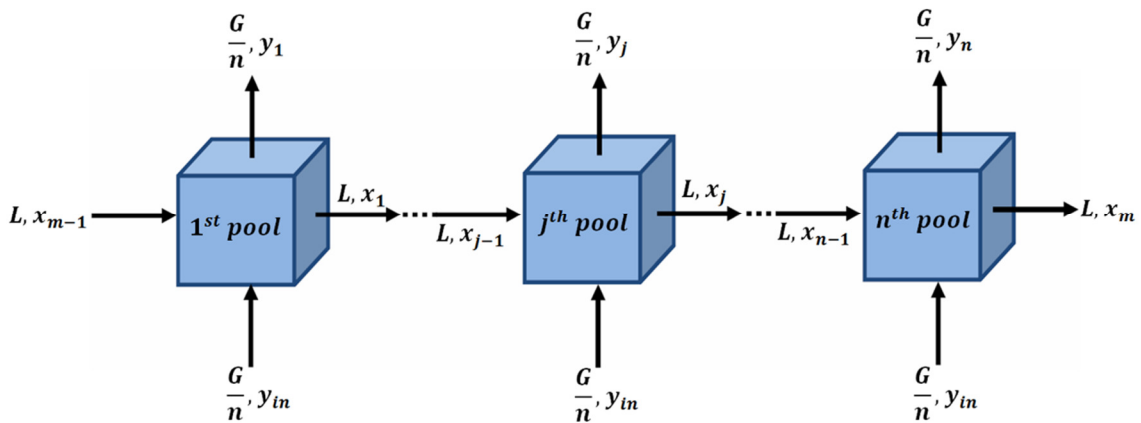
377

378 **3.2.1 Mixed Stages Model**

379 Gautreaux and O’Connell<sup>64</sup> employed the Kirschbaum’s idea of perfectly mixed stages on separa-  
 380 tion trays. They revisited the mixed pool concept and derived the equation

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

381 for  $n$  number of pools through material balancing on each stage (see Fig. 9), using the assump-  
 382 tions similar to the Lewis’ case I except for liquid mixing. The derivation of the tray efficiency is  
 383 simple and can be found in this publication.<sup>64</sup> The utility of this model was validated for the data  
 384 obtained from a natural gasoline fractionator<sup>65</sup> (propane-butane system).<sup>64</sup>



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

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

394 Initially, the determination of the number of pools equivalent to the actual liquid mixing in the  
 395 flow direction was unclear. Miyauchi and Vermeulen<sup>66</sup> identified the mathematical analogy be-

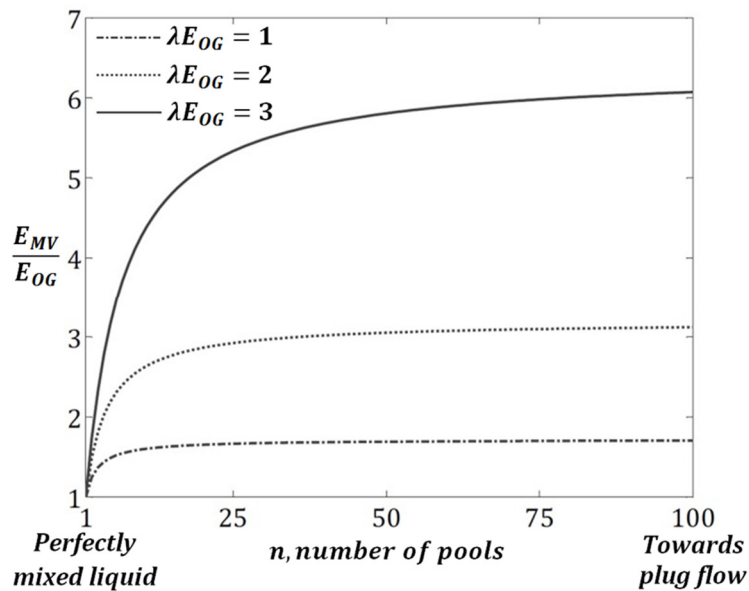


396 between the axial dispersion model and the pool model assimilating backmixing amidst two con-  
 397 secutive pools.<sup>67</sup> The parameters for quantifying the liquid mixing are Péclet number ( $Pe$ ) and  
 398 number of pools in the dispersion model and the pool model, respectively.  $Pe$  and  $n$  denote con-  
 399 tinuous and discrete mixing in the respective methods. Further, Ashley and Haselden<sup>68</sup> con-  
 400 firmed that the axial dispersion and the pool model are equivalent for

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

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

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



402

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

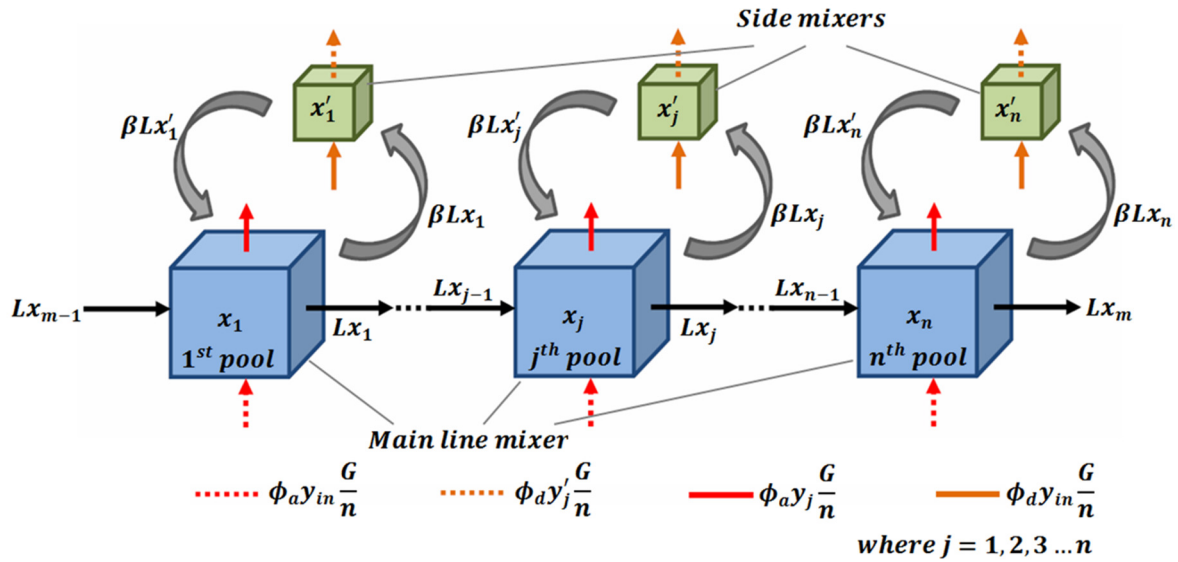
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405

### 3.2.2 Pool Cascade Model

406 Bruin and Freije<sup>67</sup> formulated a simple and versatile ‘ready-to-use’ model to incorporate the  
 407 effects of channeling and stagnant regions on the tray efficiency. Here, the term versatility refers  
 408 to the applicability of this method to a single-pass cross-flow tray of any design. This approach  
 409 assumes the tray to be comprised of a cascade of identical mixing cells called main line mixers.  
 410 This is different to Kirschbaum’s concept, as each cell has a stagnant region in the form of a side

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



415

416

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

447 the definition given by AIChE's bubble tray design manual<sup>69</sup> as

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

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

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

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

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

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

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

454 calculations. The readers are referred to these publications<sup>22,29,71-79</sup> for further information on

455 the degree of liquid mixing on trays.

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

457 as they can provide the relative size of active and stagnant regions (i.e.  $\phi_a$  and  $\phi_d$ ). To derive

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

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

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

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

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

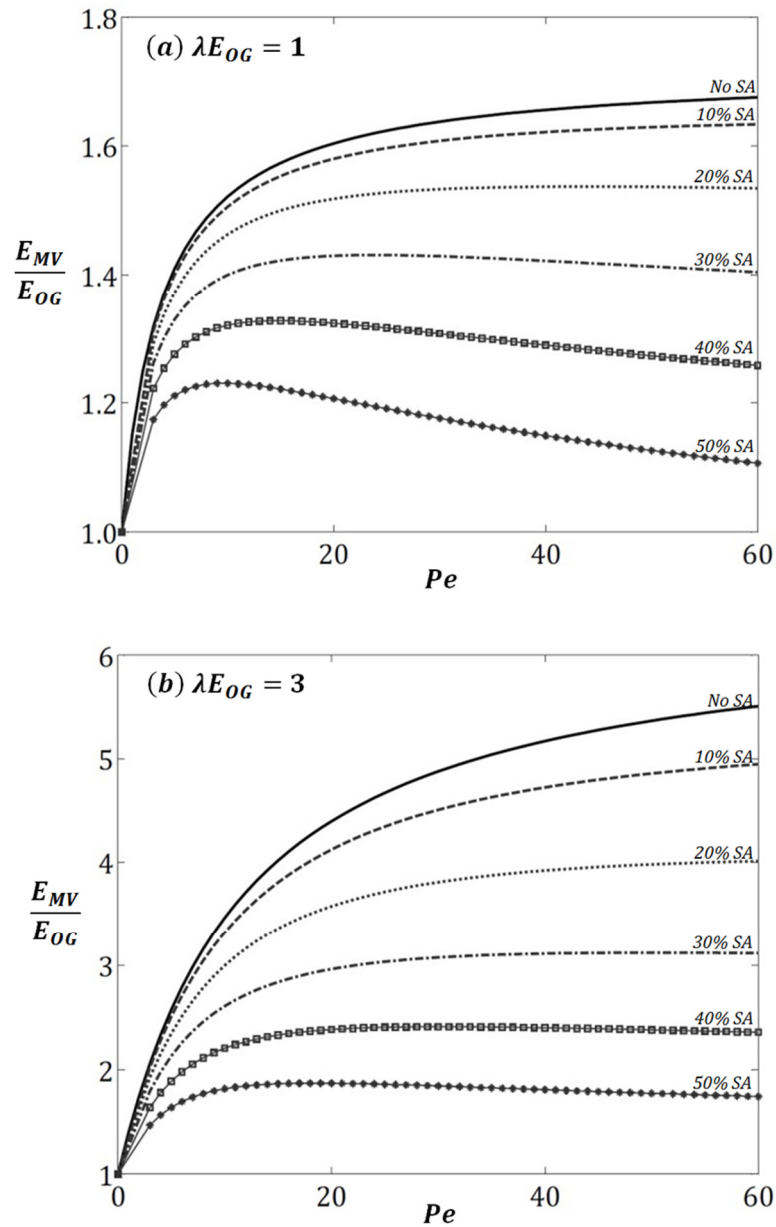
463 yield

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

464 The term  $\beta_o$  is an empirical fitting parameter and can be treated like a constant. This parameter  
 465 can be calculated by using the above equation in conjunction with Eq. 20 for a system with  
 466 known efficiencies. Bruin and Freije<sup>67</sup> recommended this parameter to be 4 as a first approxima-  
 467 tion and validated the accuracy of this model through experimental data (Zuiderweg et al.<sup>80</sup> and  
 468 Gerster et al.<sup>74</sup>) and the eddy diffusion model<sup>21</sup> (discussed in Section 3.3.2). The current model is  
 469 in good agreement with the Porter's model<sup>21</sup> but generally over-calculates the efficiencies by  
 470 approximately 5-10% compared with the experimental data.

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

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



489

490

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

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

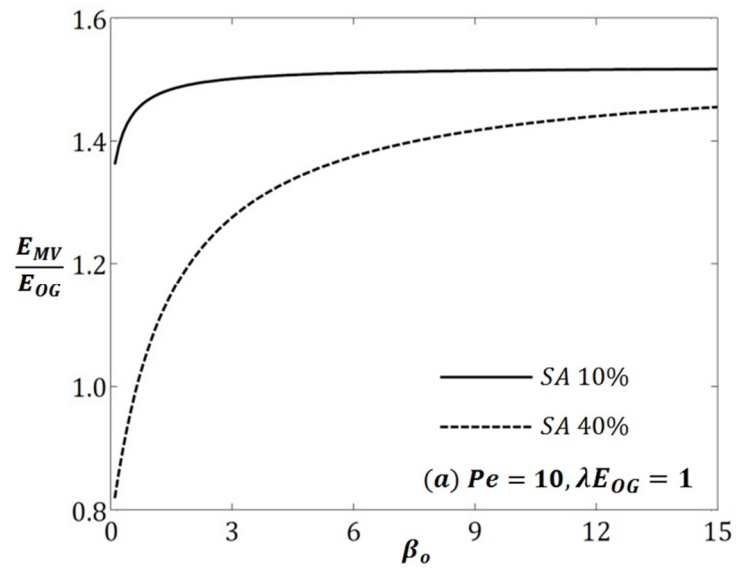
493 In Fig. 12, a sharp rise in the tray efficiency for low values of the Péclet number is visible. This  
 494 means that transverse mixing of the liquid is dominant at this instant, which equalizes any flow  
 495 non-uniformity on the tray.<sup>20</sup> In other words, the cross-flow liquid mixing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

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

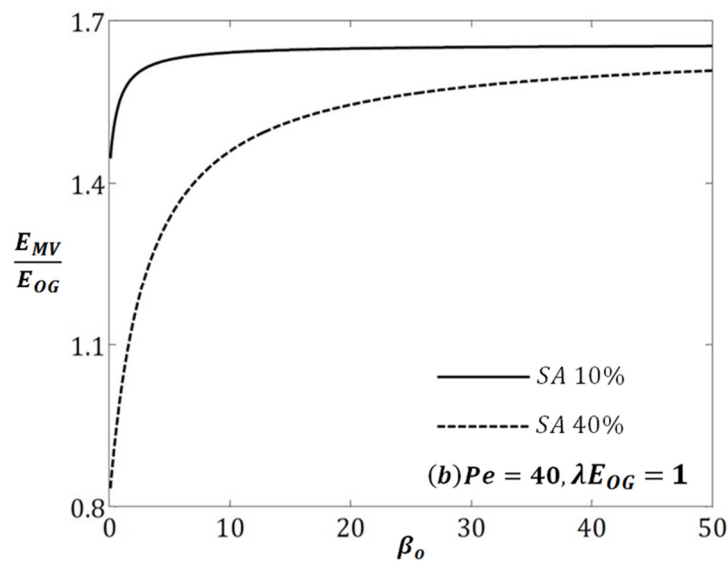
514 Fig. 13 aims at providing information on the selection of the empirical parameter  $\beta_o$  (Eq. 24) for  
515 arbitrarily chosen values of  $Pe$  (10 and 40) and  $\lambda E_{OG}$  (1). When  $Pe$  is 10, the maximum value of  
516  $\beta_o$  is 18.9, for which  $\beta$  is marginally less than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

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

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



528



529

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

531

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

532

533

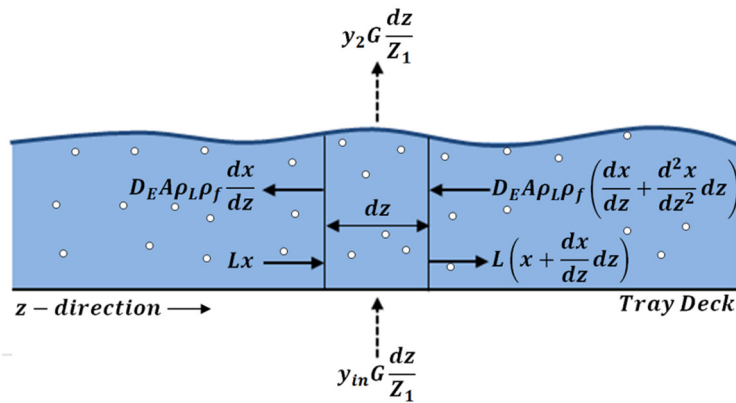
534



535 **3.3 Diffusional Models**

536 **3.3.1 AIChE Model**

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



544

545

**Fig. 14.** Schematic representation of the AIChE model.

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

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

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

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

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

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

558 The boundary conditions for the above equation are

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

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

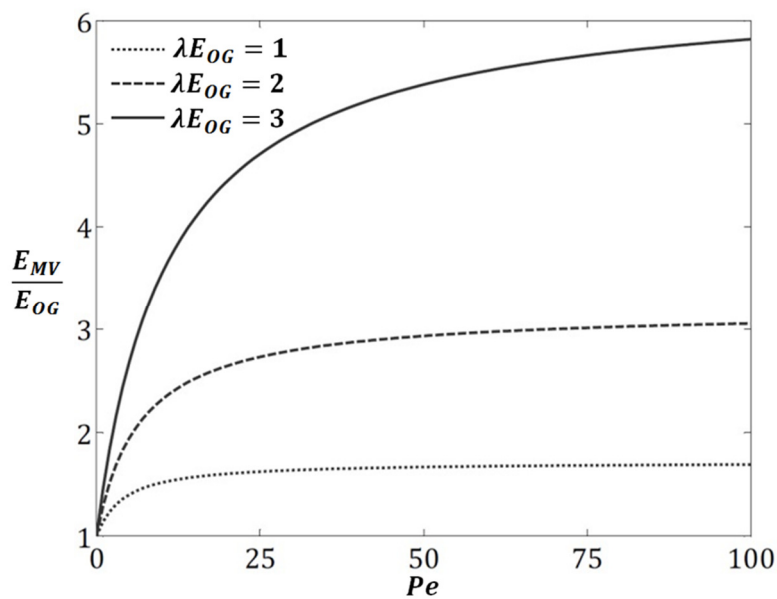
559 The second-order ordinary differential equation (Eq. 27) is solved in Appendix B for the given  
 560 boundary conditions (Eqs. 28 and 29) and the final expression for the tray efficiency is

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

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

561 Here, the tray efficiency depends on  $Pe$  and  $\lambda E_{OG}$  only, out of which  $Pe$  requires an accurate de-  
 562 termination of  $\tau$  and  $D_E$ . As already mentioned in the pool cascade model, the eddy diffusion  
 563 coefficient is influenced by the design of the tray.<sup>70</sup> The AIChE's report<sup>74</sup> gives a correlation of  
 564 this coefficient for a rectangular bubble-cap tray; however, the flow patterns on circular trays  
 565 can be very different than the idealized rectangular trays.<sup>20</sup> Further, the flow non-idealities are

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



573

574

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

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

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

595

### 596 3.3.2 Eddy Diffusion Model

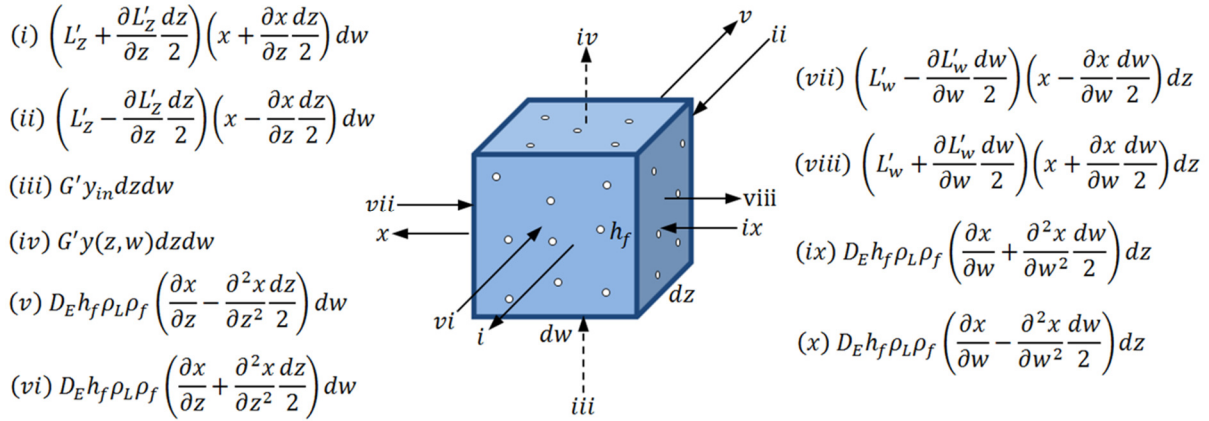
597 Porter et al.<sup>21</sup> and Lim et al.<sup>82</sup> developed the eddy diffusion model for single-pass and double-  
598 pass cross-flow trays, respectively. These models account for liquid mixing in the flow direction  
599 as well as in the transverse direction. Safekourdi<sup>58</sup> advanced these models by including liquid  
600 velocities in terms of stream function over the bubbling area of the tray. The assumptions con-  
601 sidered during the model formulation are

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

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

610 having an aerated liquid (froth) with a uniform height  $h_f$  is considered. The transfer of mass into  
 611 and out of this elemental froth is governed by the following mechanisms<sup>58</sup>:

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



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

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

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

618 Rearranging the above equation according to Appendix C gives

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

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

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

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

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

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

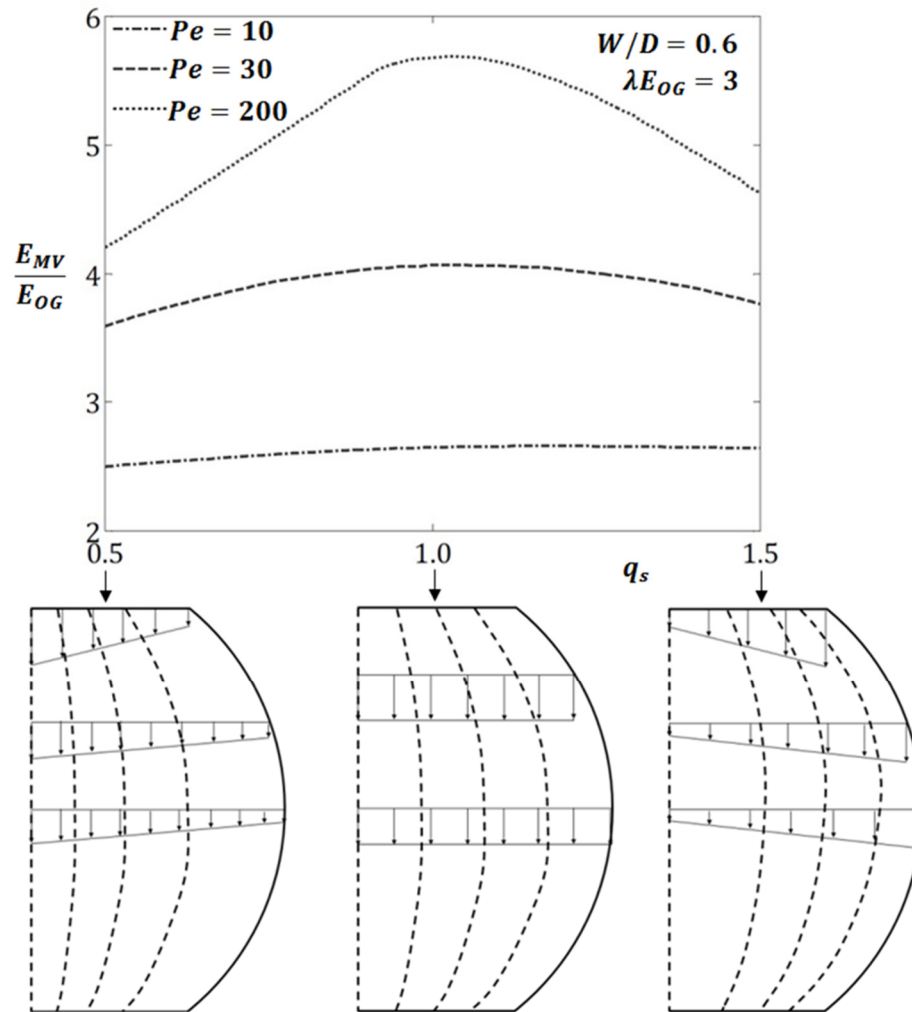
620 Eq. 33 is solved numerically with its associated boundary conditions using finite difference  
 621 method. A detailed description on the finite-difference scheme, successive relaxation method  
 622 and treatment of differentials near the wall are given in this publication.<sup>58</sup> Subsequently,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

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

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

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

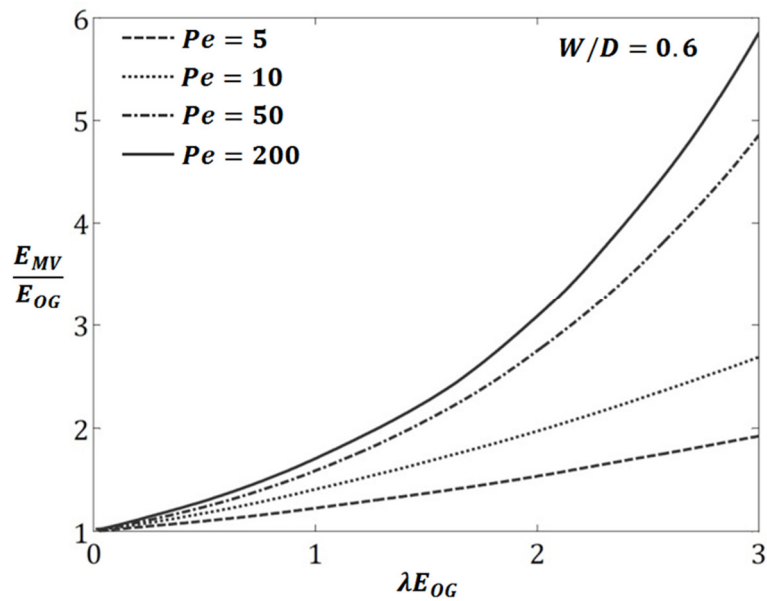
642 with the numerical solution of the AIChE<sup>69</sup> model. A slight overestimation of 3% in the efficiency  
 643 required the predictions to be corrected by this value.<sup>83</sup> All results presented in this section have  
 644 been corrected accordingly. The predictions from the model developed by Porter et al.<sup>21</sup> was  
 645 another criterion for the model authentication.



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

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

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

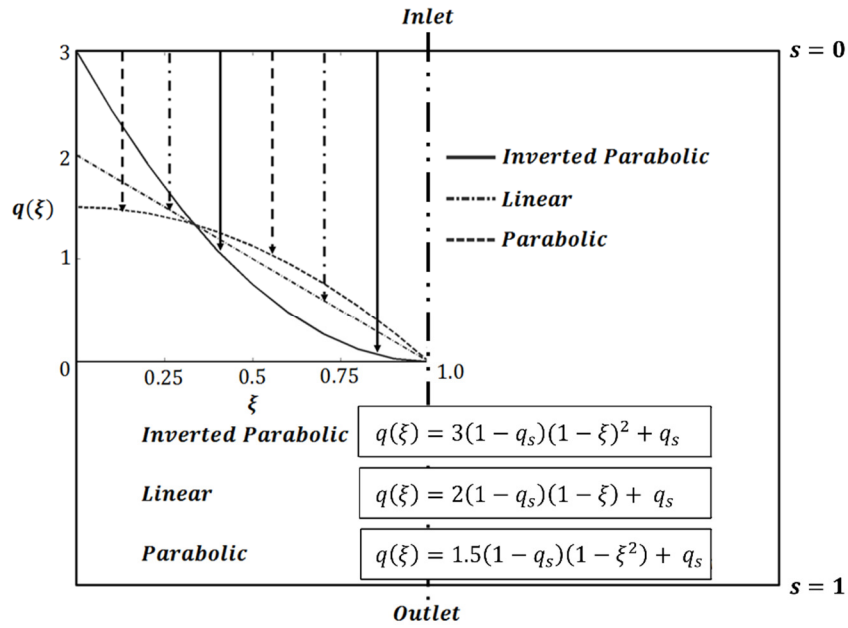


655  
656 **Fig. 18.** Tray efficiency prediction for the optimum velocity profile by the eddy diffusion model.  
657

### 658 3.4 Non-uniform Flow Model

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

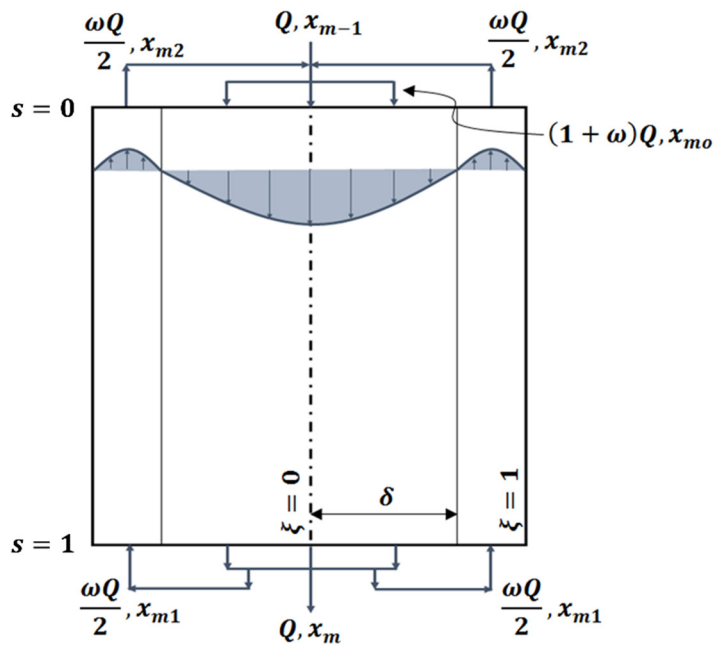




669

670

(a)



671

672

(b)

673

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

674

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

675

Bell<sup>28</sup> and Solari<sup>83</sup> reported the general mass transport equation for a binary system, derived

676

from the species continuity equation, as

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

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

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

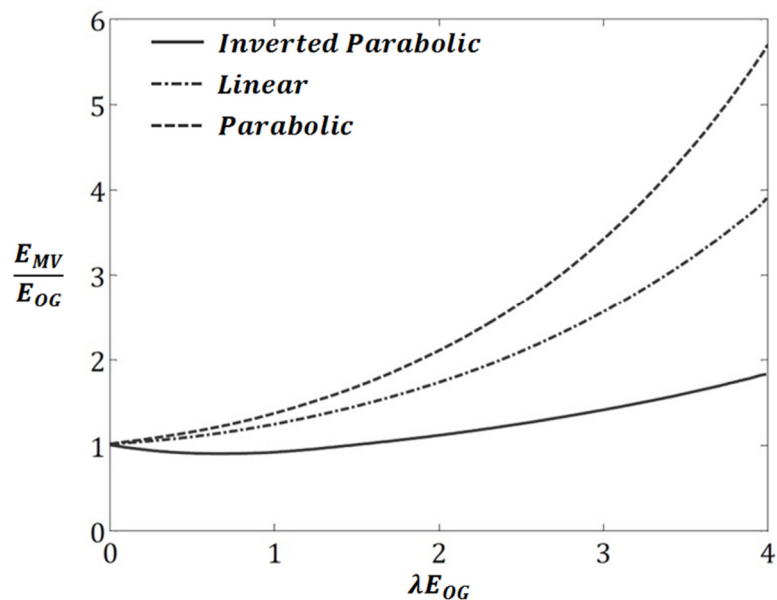
683 Eq. 40 is solved for  $x(s, \xi)$  by the method of separation of variables and subsequently used in the  
684 definitions of tray and point efficiency, which leads to

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

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

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

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



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

709 Similar to the simple non-uniform flow model, Bell and Solari<sup>84</sup> devised another model by ac-  
710 commodating a retrograde flow on either side of the forward flow path, as demonstrated in Fig.  
711 19b. The forward and the retrograde flow regions are separated by a line, where the liquid ve-  
712 locity is zero. This type of model has been termed as the ‘non-uniform retrograde flow model’  
713 and is further classified into two sub-categories. In the first model, the liquid flowing through the  
714 forward flow path is perfectly mixed at the outlet. A fraction of this uniform composition liquid  
715 is diverted to the retrograde flow path and is called as ‘uniform composition model’ (as shown in  
716 Fig. 19b). In the second model (not shown here), some of the flow paths of the liquid near zero

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

723

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

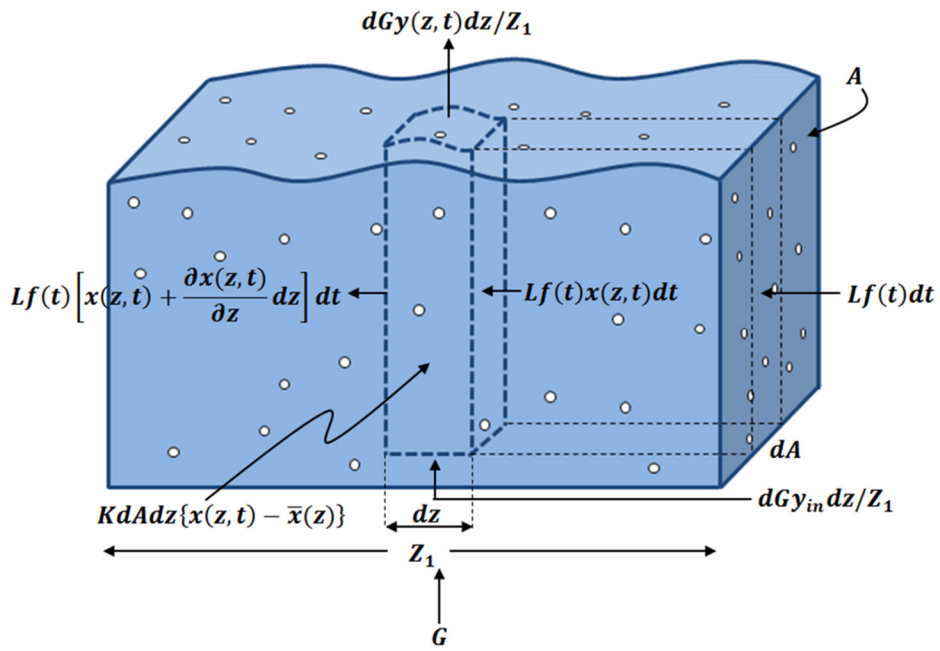
725 The RTD model employs the residence time concept to characterize the degree of liquid mixing  
726 on a tray. This method assumes that the mixing of liquid produces a distribution of residence  
727 time, ranging from zero to infinity.<sup>73,85</sup> This approach is capable of establishing the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

730 The concept of residence time is well-known and has been subjected to numerous studies in  
731 interdisciplinary fields.<sup>86-88</sup> Danckwerts<sup>89</sup> presented the unified and comprehensive treatment of  
732 this concept in continuous flow systems, after which the RTD studies gained large recognition  
733 and found application in chemical and reaction engineering. The experimental determination of  
734 the RTD based upon injection and dispersion of appropriate tracers, known as stimulus-  
735 response method, is discussed in detail in the literature.<sup>90</sup>

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

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

742 (iv) linear VLE curve.



743

744

**Fig. 21.** Schematic representation of the RTD model.

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

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

753 Similarly, the mean residence time of all streams is

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

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

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

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

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

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

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

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

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

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

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

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

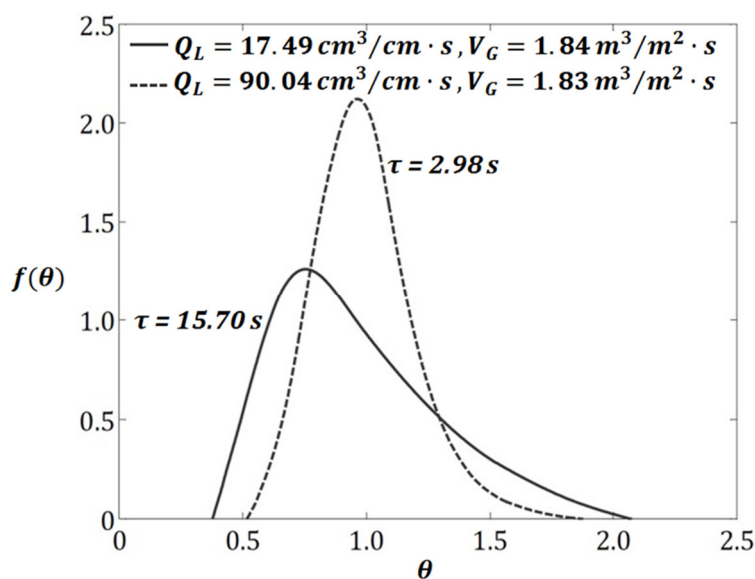
$$\frac{E_{MV}}{E_{OG}} = \frac{1 - \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt}{\lambda E_{OG} \int_0^{\infty} \exp(-\lambda E_{OG} t/\tau) \cdot f(t) dt} \quad (49)$$

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

773 The dependency of the tray fractionation efficiency on  $f(t)$  and  $\lambda E_{OG}$  is evident from Eq. 49. As  
 774 far as previous tray models are concerned, liquid mixing in the flow direction is accounted by the  
 775 Péclet number. Except for the eddy diffusion model,<sup>21,58,82</sup> no account of the Péclet number nor-  
 776 mal to the flow direction for transverse mixing has been observed. The absence of Péclet number  
 777 in this model is automatically compensated by the residence time function, as it also recognizes  
 778 the mixing in the flow direction. However, point tracer concentration measurements in stimulus-  
 779 response experiments further enable to extract the flow patterns on the trays.<sup>18,26-28</sup> The cor-  
 780 rectness of this model has been justified through the oxygen-stripping studies<sup>92</sup> on a sieve tray  
 781 unit operated with oxygen-rich water and air. The present model slightly over-predicts the effi-  
 782 ciency (approximately 5%) due to non-uniform froth conditions at the liquid entrance.<sup>73</sup>

783 There is a severe lack of data concerning the residence time function of liquid on cross-flow  
 784 trays. Foss et al.<sup>73</sup> conducted the tracer experiments on a rectangular sieve tray that was 36  
 785 inches long and 9.5 inches wide. A concentrated solution of salt was used as the tracer. A step  
 786 input of the tracer was supplied to the liquid entering the tray. The tracer concentration in the  
 787 effluent stream was measured continuously by a conductivity cell.<sup>85</sup> The residence time func-  
 788 tions with their mean residence time at different load conditions are exemplarily presented in  
 789 Fig. 22a.<sup>73</sup> The curve with the mean residence time of 15.7 s corresponds to liquid flow rate of  
 790 17.49 cm<sup>3</sup>/(cm·s) and gas flow rate of 1.84 m<sup>3</sup>/(m<sup>2</sup>·s). Similarly, the curve with the mean resi-  
 791 dence time of 2.98 s corresponds to liquid and gas load of 90.04 cm<sup>3</sup>/(cm·s) and 1.83 m<sup>3</sup>/(m<sup>2</sup>·s),

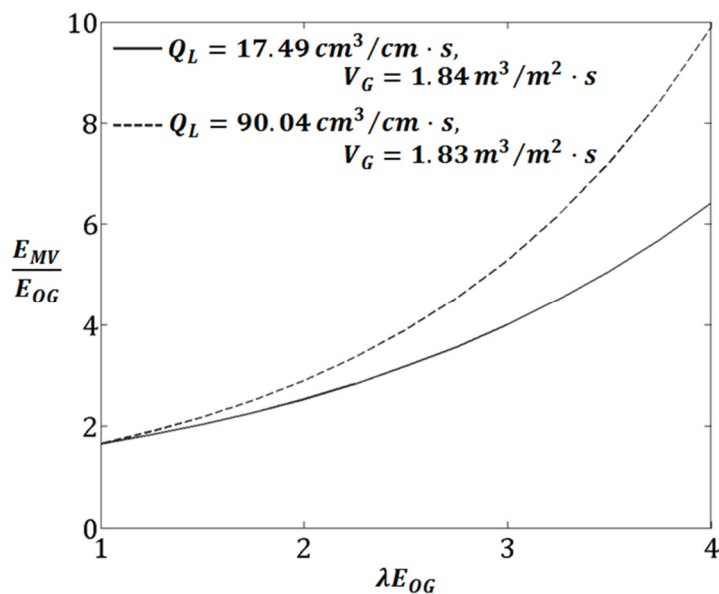
792 respectively. The liquid and gas flow rates are mentioned here with respect to the width and the  
 793 active area of the tray, respectively.



794

795

(a)



796

797

(b)

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

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



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

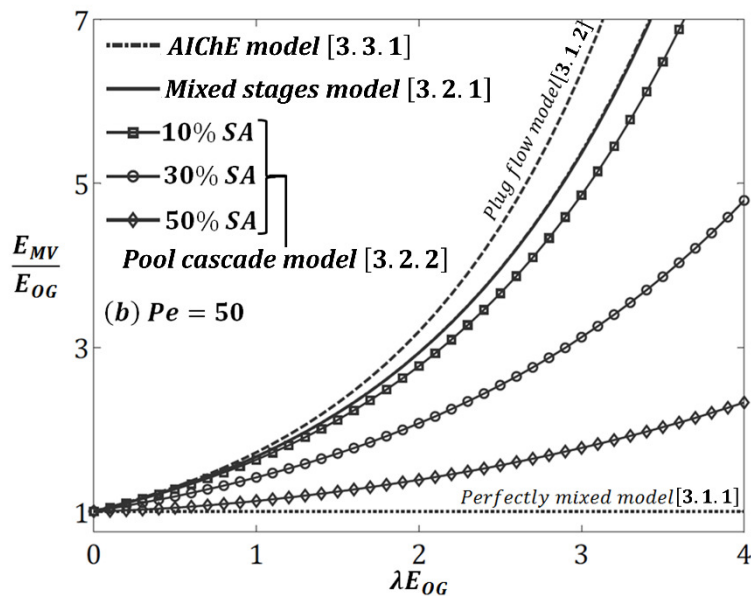
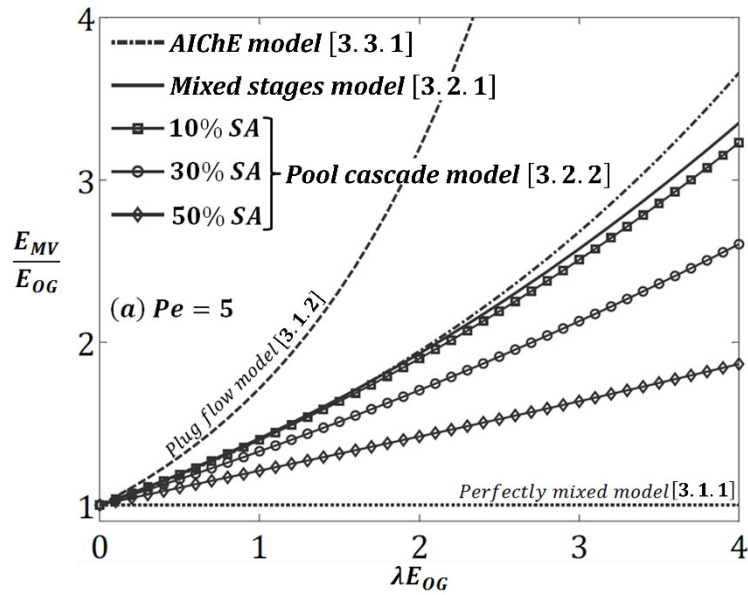
818 A weak point of the RTD studies is that they are unable to uniquely determine the nature,<sup>93</sup> as  
819 well as the location of the non-ideality. Similar tracer response is possible for different non-  
820 idealities at different locations on the tray. However, this approach is the most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

827

## 828 4. Comparison of Modeling Schemes

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

836 The plug flow [3.1.2] and the perfectly mixed [3.1.1] model provide the upper and the lower lim-  
837 its of the tray efficiency, respectively. The predictions by the mixed stages model [3.2.1] and the  
838 AIChE model [3.3.1] at  $Pe = 50$  practically coincide. These models consider the liquid backmix-  
839 ing only and are unconcerned towards the stagnant regions due to which the results from the  
840 pool cascade model [3.2.2] at  $\beta_o = 4$  are also presented. It is obvious that the size of the stagnant  
841 regions is proportional to the loss in the tray efficiency. The influence of  $\lambda E_{OG}$  and Péclet number  
842 on the tray efficiency has been discussed several times in this work. However, this model com-  
843 parison is only applicable for the tray assuming uniform liquid flow at the inlet. Apart from this,  
844 Bell and Solari<sup>84</sup> reported that the tray efficiency becomes less than the point efficiency for an  
845 inverted parabolic velocity profile of liquid at the inlet (see Fig. 20). The pool cascade model also  
846 provides similar observation (not shown here) e.g. the  $E_{MV}/E_{OG}$  ratio goes below unity for rela-  
847 tive stagnant regions larger than 80% at  $Pe = 5$ .



848

849

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

851 (b)  $Pe = 50$ .

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

859 vapor distributions in the model formulation. Further, the ‘Hybrid modeling’ approach combin-  
 860 ing experimentally validated CFD and tray efficiency models seems to be a promising alternative  
 861 for realistic efficiency predictions. Such hybrid approach could be preferred in the future as ‘vir-  
 862 tual experiment’<sup>36</sup> 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.<sup>9</sup> Lastly, the  
 865 tray efficiencies are calculated using the flow conditions at the tray boundaries, i.e. inlet and  
 866 outlet, without giving any preference to the flow scenario at intermediate locations (except in  
 867 the eddy diffusion model). This is similar to the treatment of distillation trays as black box.  
 868 Therefore, an account of the intermediate flow conditions in phenomenological models for  
 869 evolving tray efficiencies is another necessity.

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

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

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

873 One obvious question that remain unanswered is that how to utilize the experimental studies for  
874 extracting the inputs required for the mathematical models. The stimulus-response method has  
875 been a popular choice to quantify the flow patterns in process equipments, and was preferred by  
876 Solari and Bell<sup>26</sup> and Schubert et al.<sup>18</sup>, while using fibre-optic system and conductivity wire mesh  
877 sensor (WMS) respectively. The latter study is favored for the aforementioned purpose due to  
878 the availability of data at comparatively high spatial and temporal resolution. In this investiga-  
879 tion, two sieve trays with 5% fractional open area were used in an 800 mm diameter column. A  
880 WMS, comprising of two orthogonal planes of transmitting and receiving wires, was embedded  
881 on one of the trays. The effects of liquid load and outlet weir design on the flow patterns were  
882 evaluated through the dispersion of salt ( $\text{Na}_2\text{SO}_4$ ) solution used as the tracer. The virtual cross-  
883 ing points between axially separated transmitters and receivers in the WMS allow measuring  
884 time-dependent tracer concentrations, and hence point liquid residence time distribution. The  
885 readers are referred to Schubert et al.<sup>18</sup> for further details on column design, data calibration  
886 and flow visualization.

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

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

891 Here,  $C_{in}(t)$  and  $C_{out}(t)$  are the tracer concentrations that are mathematically averaged point  
892 concentrations for each time step at the tray inlet and outlet, respectively. In this work, the data  
893 from the WMS points next to the weirs are avoided to neglect the effect of non-uniform froth at  
894 the boundaries<sup>73</sup>, as well as to account for the flow in the tray bubbling area only. These bounda-  
895 ries will be referred as WMS boundaries hereafter. Furthermore, the symbol  $\otimes$  refers to the

896 convolution integral, whose calculation is straightforward.<sup>90,94</sup> The converse of this integral is  
 897 called deconvolution, which is challenging and hence requires special approaches.<sup>94</sup> 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.<sup>90,94-108</sup> The cit-  
 900 ed literature also explains the pros and cons of these techniques due to which they are not dis-  
 901 cussed here. The model fitting approach is preferred in this work, because of the computational  
 902 ease due to the availability of the standard RTD function from the axial dispersion model. The  
 903 WMS boundaries permit to use the Gaussian function for the open-open boundary  
 904 condition<sup>90,101,109</sup> as

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

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

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

911 This generalized definition of  $Pe$  is apt for the open-open boundary condition. For the closed  
 912 system, the mean residence time is the same as the hydraulic time.<sup>90,91</sup> This is an explanation for  
 913 the appearance of the mean residence time in Eq. 23 as proposed in the AIChE manual<sup>69</sup>.

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  $\tau_h$ , 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  $\tau_h$  for a good agreement between the actual and the convo-  
 923 luted function.<sup>110</sup>

924 Further, the mean residence time can be obtained from the hydraulic time in the open-open sys-  
 925 tem<sup>90</sup> as

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

926 while the other definition of  $\tau$  is given by Eq. D3 in the Appendix D. The residence times obtained  
 927 from Eq. 54 and D3 are consistent, which proves the validity of the RTD function as well as of  
 928 this algorithm. The rationality of this algorithm can be further justified by the consistency of the  
 929 RTD variances according to<sup>90</sup>

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

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

930 The estimation of the RTD enables computing the relative active and stagnant volumes on the  
 931 tray. Duduković and Felder<sup>111</sup> suggested the tail of the impulse response function, accountable  
 932 for the stagnant volume, to be truncated to acquire the active volume. Such truncation is re-  
 933 searcher's perception dependent, and can lead to inconsistent fractions. Sahai and Emi<sup>112</sup> pro-  
 934 posed that any fluid staying in a system for a period longer than twice the mean residence time

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

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

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

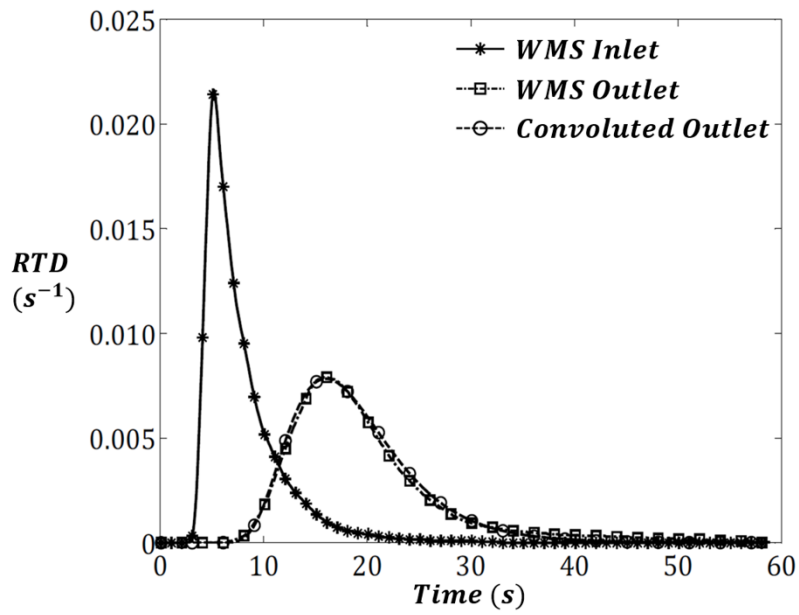
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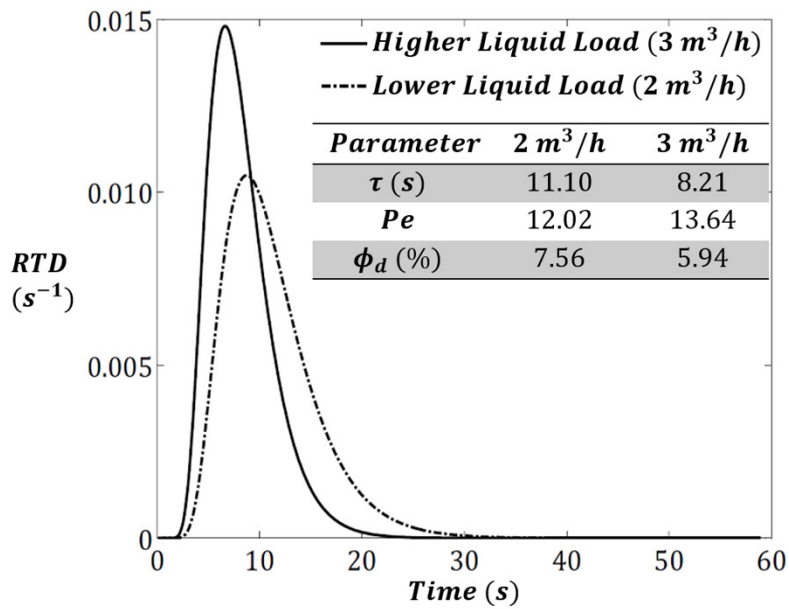
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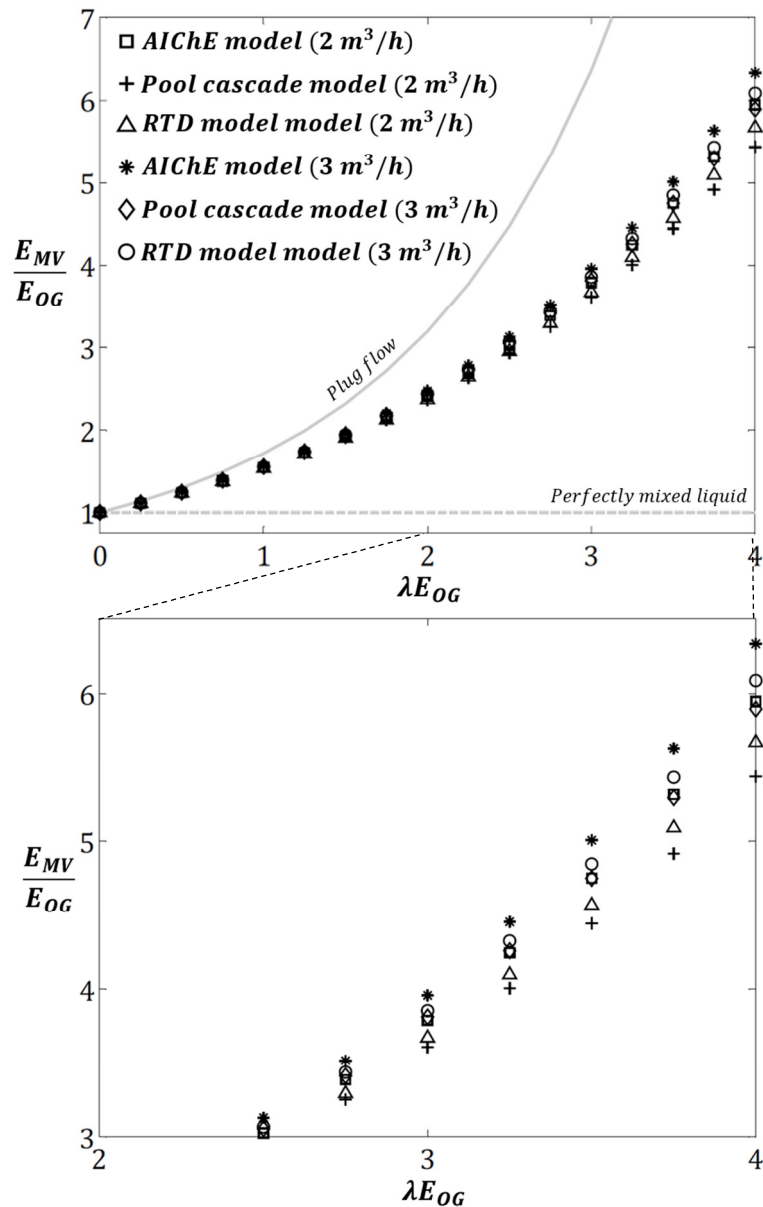


(a)



(b)

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



957

958  
959  
960

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

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

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

978

## 979 **6. Concluding Remarks and Perspective**

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

995 models has been presented by stating their formulation, strengths, weaknesses and associated  
996 analysis. Also, the dependence of the tray efficiency on system and flow properties has been  
997 discussed. Furthermore, a concise algorithm concerning the processing and utilization of the  
998 experimental data in tandem with mathematical models has been proposed. This work is 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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1005

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1008

## 1009 **8. Nomenclature**

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

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

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

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

1080

1081 **Subscripts**

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

1095

1096 **Superscript**

1097	*	Equilibrium
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1098 **Greek Letters**

1099	$\beta$	Fraction of liquid that circulates between main line mixer and side mixer (-)
1100	$\beta_o$	Empirical fitting parameter in the pool cascade model (-)
1101	$\gamma$	Parameter used in the plug flow model (-)
1102	$\delta$	Central tray area with forward flow per total tray area (-)
1103	$\eta$	Parameter used in the AIChE model (-)
1104	$\theta$	Non-dimensional time (= $t/\tau$ ) (-)
1105	$\lambda$	Stripping factor (-)
1106	$\xi$	Non-dimensional distance from the tray centerline orthogonal to the flow direction (-)
1107		
1108	$\rho_L$	Clear liquid density (kmol/m <sup>3</sup> )
1109	$\rho_F$	Froth density (= volume of liquid/froth volume) (-)
1110	$\sigma^2$	Variance of the RTD function (s <sup>2</sup> )
1111	$\tau$	Mean residence time of the liquid on the tray (s)
1112	$\tau_h$	Hydraulic or space time (= volume of the system/volumetric flow rate) (s)
1113	$\phi_a$	Relative volume of the active region in the pool cascade model (-)
1114	$\phi_d$	Relative volume of the stagnant region in the pool cascade model (-)
1115	$\psi$	Stream function (m <sup>2</sup> /s)
1116	$\psi_o$	Stream function value at the column wall (m <sup>2</sup> /s)
1117	$\omega$	Fraction of the recycled liquid as retrograde flow (-)

1118

1119 **Abbreviations**

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



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

1131

## 1132 **Appendix (A)**

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

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

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

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

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

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

1136 Using the binomial expansion, one can write

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

1137 The application of the limit in Eq. A3 provides

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

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

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

1139

## 1140 **Appendix (B)**

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

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

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

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

1143 The solution of Eq. B1 is given by

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

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

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

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

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

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

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

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

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

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

1147 Earlier, it has been stated that

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

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

1149 permits to formulate the tray efficiency as

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

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

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

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

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

1151

1152 **Appendix (C)**

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

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

1154 The equation of continuity is

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

1164

## 1165 **Appendix (D)**

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

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

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

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

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

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

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

1170 The mean residence time is defined as

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

1171 Using Eq. D3, Eq. D2 transforms to

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

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

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

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

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

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

1175 The Murphree efficiency for the liquid-side is

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

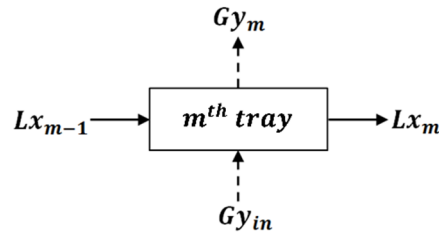
1176 The average composition of liquid exiting the tray can be found using Eq. D6 as

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

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

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

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



1179

1180

**Fig. D1.** Material balance over the tray boundaries.

1181

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

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

1182

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

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

1183

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