A Novel RTD Compartment Model for Tray Efficiency Predictions

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In the present work, a new model built through refinement of the existing residence time distribution model [Foss, PhD Thesis, University of Delaware, 1957] is proposed. In this new model, the tray is imaginarily partitioned into compartments along the liquid flow direction between inlet and outlet. This partitioning allows computing the tray efficiency through quantification of the efficiencies of the individual compartments. Therefore, the fluid dynamics of each compartment contribute towards the evolving tray efficiency, thereby breaking the tray's black-box convention. The tray segmentation further supports in studying the effects of vapor maldistribution as well as flow path length on the tray efficiency. This indicates the versatility and advantage of the new model over the existing ones. In particular, the mathematical formulation of this model along with its theoretical validation and application through analysis of suitable case studies are presented.

1. Introduction

Distillation is the most applied thermal separation technology in chemical process industries accounting for 95% of all worldwide separation duties (Chuang and Nandakumar, 2000). Distillation columns are energy-intensive process equipments responsible for 3% of the global energy consumption (Masoumi and Kadkhodaie, 2012). Approximately half of these columns in the world are and will be equipped with trays (Górak and Olujić, 2014). The single-pass cross-flow tray is the most common tray configuration in these columns. The evolving flow patterns on these trays strongly dictate their (Murphree) efficiency (i.e. the ratio between the actual change in average vapor/liquid composition on the tray over the composition change for an equilibrium stage) as well as overall performance of the column. Plug flow of liquid and vapor are considered ideal for the tray efficiency (Górak and Olujić, 2014). Any deviation from plug flow is called non-ideal flow or simply maldistribution, which is known for deteriorating the tray performance. Liquid flow patterns on cross-flow trays are complicated and far from plug flow, due to the agitation caused by rising vapor, dispersion, and expanding and contracting flow path (because of circular cross-section of the column) (Górak and Olujić, 2014). Experimental studies have revealed liquid maldistribution on the trays, such as channeling, recirculation, retrograde flow and presence of stagnant regions. In particular, tracer dispersion experiments have been preferred to determine the flow and mixing patterns of liquid on the trays. In these experiments, the residence time distribution (RTD) of liquid is obtained through dispersion of tracer (e.g. salt or dye solution) that is injected at the inlet as instantaneous pulse or step. Mostly, conductivity probes and fiber-optic probes are used for transient sampling of the tracer exiting a tray. Recently, Schubert et al. (2016) used wire-mesh sensor (WMS) to obtain the point liquid RTD across a sieve tray for various liquid loads and weir designs at high spatio-temporal resolution.

In the literature, mathematical models were formulated to predict the tray efficiency based on flow and mixing patterns on a tray. The existing models, recently revisited by Vishwakarma et al. (2018), rely on parameters for which tracer sampling is only required at the tray outlet. These models are unable to employ any flow information at intermediate tray locations along the liquid flow path. This procedure of efficiency prediction suggests the perception of tray as a black box, despite of recent advancements in measuring and imaging techniques. In addition, uniform vapor load on a tray is assumed in these models, which is only possible on

either small trays or the lowest tray in a column next to reboiler (Lockett and Dhulesia, 1980). Excessive liquid gradients on a tray can cause serious non-uniform distribution in the vapor flow, and vice-versa (Mohan et al., 1983). Further, the vapor also attempts to by-pass the column through stagnant liquid pools, if these pools are piled over one another near the column wall. So far, only few authors have managed to study the effects of non-ideal vapor flow on the tray efficiency through modification of the existing models. Lewis (1936) and Diener (1967) reported the effects of unmixed vapor rising in a column on the tray efficiency during plug flow and partially mixed flow of liquid, respectively. Later, Ashley and Haselden (1970) studied the influence of partial vapor mixing between the trays, using mixed pool approach, on the tray efficiency. However, none of these studies considered non-uniform flow of vapor through the trays. On the other hand, Furzer (1969) observed the reduction in tray efficiency during dispersed liquid flow and linearly distributed vapor flow along the tray. The linear vapor distribution was reported to have no effect on the tray efficiency during perfectly mixed and plug flow of liquid. Lockett and Dhulesia (1980) also concluded that the tray efficiency is insensitive to vapor maldistribution during plug flow of liquid. However, Mohan et al. (1983) reported that the vapor maldistribution is detrimental to the tray efficiency during plug flow and perfectly mixed flow of liquid. Such disagreement in tray efficiency predictions even during the ideal cases of liquid flow reflects the scarcity of scientific work in this regard. Besides, different degrees of non-uniformities may exist in the vapor flow due to varying liquid load and tray design, which would affect the tray performance accordingly. This motivates towards studying the impact of liquid as well as vapor maldistribution on the tray efficiency.

The present work proposes a new model that is formulated through refinement of the existing RTD approach (Foss, 1957). The refined model is capable of accounting the impact of flow non-uniformities in both phases on the tray efficiency. In addition, the effect of flow path length on the tray performance can also be studied using this model, thereby indicating the versatility and advantage of this model over the existing ones. In this work, the mathematical formulation of the new model, its theoretical validation and application through analysis of suitable case studies are presented. Mathematical processing of the tracer concentration profiles to obtain the liquid RTD function is also discussed in this work.

2. Model description

2.1 Background

The RTD model (Foss, 1957) uses the theory of residence time by presuming that the mixing of liquid on a tray results in distribution of liquid residence times, theoretically ranging from zero to infinity. This model assumes that the liquid stream consists of infinite separate streams, each with a definite residence time, on a tray. The liquid composition in each stream is affected by mass transfer to the vapor, according to the local point efficiency (E_{OG}), and by mass exchange with the surrounding liquid. Plug flow of vapor, complete liquid mixing along the froth height, and linear vapor-liquid equilibrium (VLE) are further considered in the RTD model. Thus, the total material balance (by integrating the material balance on differential fluid elements) over a tray for a given liquid RTD function $f(t)$ results in the RTD model as

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

E_{MV} is the vapor-side tray efficiency, τ is the mean residence time of liquid, while λ is called as stripping factor (i.e. the ratio of VLE and operating lines for a tray). Foss (1957) validated this model through oxygen-stripping experiments on a rectangular sieve tray operated with oxygen-rich water and air. If the point efficiency is assumed as constant, the rearrangement of the above equation allows using Laplace transform as

$$\int_0^\infty exp\left(-\frac{\mu t}{\tau}\right) \cdot f(t)dt = F\left(\frac{\mu}{\tau}\right) = \frac{1}{1 + \mu\frac{E_{MV}}{E_{OG}}}\ . \tag{2}$$

In Eq(2), F is the Laplace function, while μ is the dimensionless group λE_{OG}. The readers are referred to the PhD thesis of Foss (1957) for further description of this model.

2.2 Formulation of the refined model

A significant improvement in the RTD model is possible through fictitious division of a tray into compartments in the liquid flow direction as shown in Figure 1a. In this figure, the tray is divided into 'n' compartments, where each compartment is separated by the boundaries termed as 'dividers'. It is imagined that liquid flows through these compartments amidst weirs, while the vapor rises through these compartments in the upward direction perpendicular to the horizontal plane. Such partitioning of tray into compartments is similar to the mixed pool model (Gautreaux and O'Connell, 1955), except the existence of perfectly mixed liquid pools with uniform

vapor distribution in the latter model. Each of these compartments are presumed to act like a cross-flow tray with unique RTD and the efficiency according to Eq(1). Analogous to the standard RTD model, following assumptions are considered to formulate the new model:

(1) Liquid stream consists of infinite separate streams, each with a specific residence time in the compartments,

(2) Plug flow of vapor in the compartments, however, the share of their flow rates in the compartments can vary,

(3) Constant point efficiency on the tray,

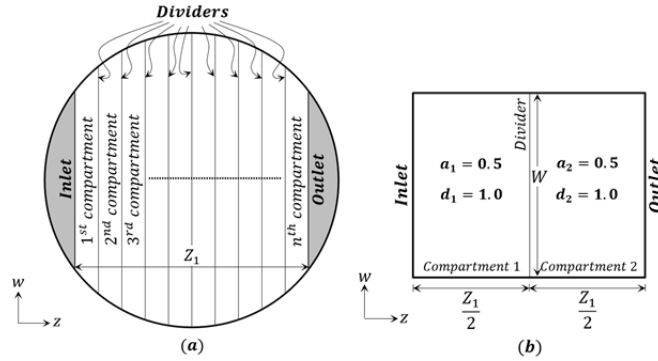(4) Complete mixing of liquid along the froth height, and

(5) Linear VLE.

Figure 1: (a) Partitioning of tray into compartments, and (b) geometrical framework of a bisected rectangular tray during uniform vapor flow.

Considering steady-state operation, the liquid and vapor flow rates in the compartments can be assumed constant as

$$L_i = L \text{ , and} \tag{3}$$

$$V_i = a_i d_i V \text{ .} \tag{4}$$

The parameters a_i (= compartment area/tray active area) and d_i are introduced as the fractional area and the vapor allocation index of the ith compartment, respectively for $i = 1, 2, \ldots n$. The mathematical conditions for these parameters are $\sum a_i = 1$, $\sum d_i = n$ and $\sum(a_i \cdot d_i) = 1$. As each compartment has a unique RTD, the summation of $L f_i(t) dt$ while material balancing (similar to the RTD model) will consider all liquid streams in a compartment. Further, the division of total vapor flow among compartments based on their fractional area and allocation index is also appropriate. The vapor allocation index is unity for uniform vapor flow in the compartments. Any other distribution of this index in the compartments would represent vapor maldistribution on the tray. Further, the assumption of constant point efficiency over the tray is also reasonable, as the point efficiency is a weak function of the superficial vapor velocity (Lockett and Dhulesia, 1980). Using Eq(2) to Eq(4), it is possible to write

$$\lambda_i = m \frac{G_i}{L_i} = a_i d_i \lambda \text{ , and} \tag{5}$$

$$\int_0^\infty exp(-\lambda_i E_{OG} \, t/\tau_i) \cdot f_i(t) dt = \frac{1}{1 + \lambda_i E_{MV,i}} \text{ .} \tag{6}$$

Here, $f_i(t)$, τ_i and $E_{MV,i}$ are the liquid RTD function, mean residence time and RTD efficiency of the ith compartment, respectively. Following mathematical treatment similar to the RTD model (not shown here), and using Laplace transform in Eq(6) produces

$$F_i\left(\frac{\mu}{\tau}\right) = \frac{1}{1 + a_i d_i \mu \frac{E_{MV,i}}{E_{OG}}}, \tag{7}$$

where F_i is the Laplace function for the ith compartment. Besides, the tray RTD function is related with the compartmental RTD functions (Levenspiel, 1999) as

$$f(t) = f_1(t) \otimes f_2(t) \otimes \cdots f_n(t) \,. \tag{8}$$

The Laplace transform of the above equation followed by the application of Eq(2) and Eq(7) results in the new model as

$$\frac{E_{MV}}{E_{OG}} = \frac{1}{\mu}\left[\left\{\prod_{i=1}^{n}\left(1 + a_i d_i \mu \frac{E_{MV,i}}{E_{OG}}\right)\right\} - 1\right] \,. \tag{9}$$

The dependence of tray efficiency on the fluid dynamics of individual compartments, through their efficiencies, is apparent in the new model. Since the tray efficiency is known for plug flow and perfectly mixed flow of liquid, the validity of Eq(9) can be assured by verifying its transformation for these ideal cases during uniform vapor load. For perfectly mixed liquid in the compartments, Eq(9) changes to the mixed pool model (Gautreaux and O'Connell, 1955). On the other hand, the new model converts to the plug flow model (Lewis 1936) during plug flow of liquid in the compartments. Further, the new model again transforms to the plug flow model for liquid plug flow with non-uniform distribution of vapor in the compartments. This can be confirmed mathematically by considering different d_i in the compartments (with individual plug flow efficiencies) in Eq(9), which indicates the consistency of this model with the studies of Furzer (1969) and Lockett and Dhulesia (1980). Thus, the proposed model given as Eq(9) is hereby validated by considering the ideal flow scenarios.

3. Case studies, results and analysis

For simplicity, a rectangular tray ($W \times Z_1$) divided into two identical and independent compartments is considered as shown in Figure 1b. For uniform distribution of vapor on this tray, the area fraction and the vapor allocation index in the compartments are 0.5 and 1, respectively. Both of these compartments are assumed to behave like a cross-flow tray with distinct RTD and efficiency according to Eq(1). Furthermore, the time-varying tracer concentration needs to be assigned at the compartment boundaries to realize the RTD function in the compartments. For instance, the tray RTD function can be calculated using the inlet ($c_{in}(t)$) and outlet tracer ($c_{out}(t)$) profiles as

$$c_{out}(t) = f(t) \otimes c_{in}(t) \,. \tag{10}$$

The inspiration for tracer concentration at the tray boundaries is taken from the WMS studies of Schubert et al. (2016). Moreover, the standard RTD function through solution of the axial-dispersion model (ADM) for open-open boundary condition is available in the literature (Levenspiel, 1999) as

$$f(t) = \sqrt{\frac{Pe}{4\pi \cdot t \cdot \tau_h}} \cdot exp\left\{-\frac{Pe\left(1 - \frac{t}{\tau_h}\right)^2}{4\left(\frac{t}{\tau_h}\right)}\right\} \,. \tag{11}$$

By assuming suitable Péclet number (Pe) and hydraulic time (τ_h), i.e. $f(t)$ in the first compartment, any tracer profile can be assigned to the divider using convolution integral similar to Eq(10). However, the divider and outlet tracer profiles are deconvolved to acquire the RTD function in the second compartment. The non-linear least square curve-fitting method is used for this purpose. In this method, the parameters Pe and τ_h in Eq(11) are iteratively modified for the second compartment, until the convolution integral of its RTD function and the divider profile is consistent with the outlet tracer profile. The correctness of the calculated RTD function can be ensured through the criteria mentioned in Table 1. The mean residence time (τ) and variance (σ^2) of the RTD function must be consistent with their definitions given for the ADM. The RTD function itself can be verified through the tanks in series model (Levenspiel, 1999), where the number of tanks depends on Pe. Furthermore, the RTDs considered in this work are presumed to persist on the tray during the assumed values of the dimensionless group λE_{OG}. This relieves from assuming L, V, m and E_{OG} separately for the tray.

Pe and τ for the bisected tray (Figure 1b) are selected as 20 and 22 s, respectively. Three different concentration profiles are assigned to the divider by assuming these parameters as well as using the aforementioned procedure. These parameters and the RTD function (not shown here) are verified using the criteria discussed in Table 1. The numerical values of these parameters are given in Figure 2a. Case I represents uniform liquid mixing in the compartments, where Pe and τ are same. Case II presents lower liquid mixing in the first compartment and comparatively higher liquid mixing in the second compartment, which is apparent from the steep divider concentration profile in Figure 2a. In Case III, liquid mixing is higher in the first compartment compared to the second compartment, as evident from the short and dispersed divider profile in Figure 2a. The tray efficiency predictions for these cases are shown in Figure 2b using their RTD functions as well as Eq(1) and Eq(9) for the assumed values of λE_{OG}. The efficiency predictions based on the RTD model

coincide with the Case I of the new model. Thus, the RTD model and the new model are equivalent to each other during uniform liquid mixing in the compartments. Further, the new model predictions during Case II and Case III are higher and lower than the RTD model predictions (of the unsegmented tray), respectively. This is because the new model is sensitive to the liquid RTD in each of the tray compartments, unlike the RTD model that depends on the RTD function of the unsegmented tray only. The difference between the predictions of the RTD model and the new model is highest at $\lambda E_{OG} = 4$. At this λE_{OG}, the new model predicts approximately 33% higher and 16% lower efficiencies than the RTD model during Case II and Case III, respectively.

Table 1: Validating criteria for deconvolution calculations.

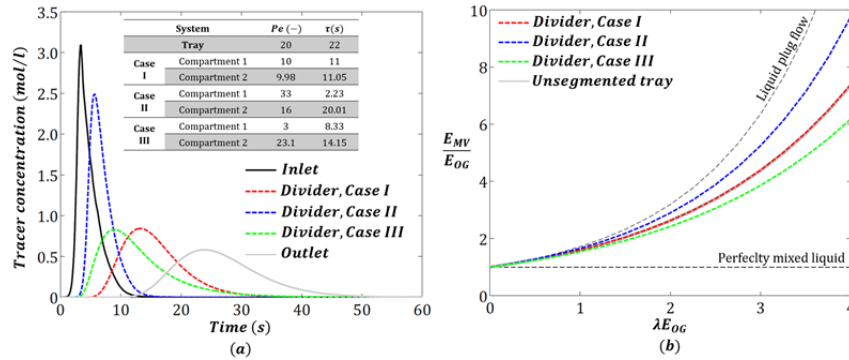| Term	Usual definition	ADM, open-open system
τ	$\int_0^\infty t \cdot f(t)dt$	$\tau_h \cdot \left(1 + \dfrac{2}{Pe}\right)$
σ^2	$\int_0^\infty (t - \tau)^2 \cdot f(t)dt$	$\tau_h^2 \cdot \left(\dfrac{2}{Pe} + \dfrac{8}{Pe^2}\right)$
$f(t)$	$\dfrac{t^{n-1}}{\tau^n} \cdot \dfrac{n^n}{(n-1)!} \cdot exp\left(-\dfrac{nt}{\tau}\right)$	Tanks in series model, where $n = \left\lceil 1 + \left(\dfrac{Pe}{2}\right)\right\rceil$

Figure 2: (a) Tracer concentration at compartment boundaries and (b) tray efficiency predictions for bisected tray during $Pe = 20$ and $\tau = 22\ s$.
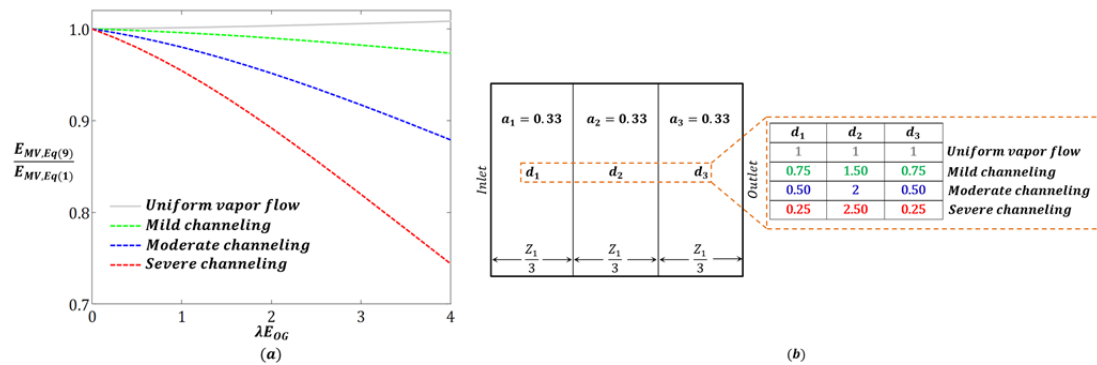

Figure 3: (a) Effect of vapor channeling on tray efficiency and (b) description of vapor allocation indices in compartments of a trisected tray during $Pe = 30$ and $\tau = 18\ s$.

To study the effect of vapor maldistribution on the tray efficiency, a trisected tray with different vapor allocation indices in the compartments (shown in Figure 3b) is considered. Uniform liquid mixing in the compartments is selected for this tray with Pe and τ as 30 and 18 s, respectively. Following the same procedure as earlier, the ratio of the predictions of the new model (Eq(9)) and the RTD model (Eq(1)) is presented in Figure 3a. It is clear that the efficiency deterioration is proportional to the degree of vapor channeling. At $\lambda E_{OG} = 4$, the difference between the predictions from the RTD model (considering only uniform vapor flow) and the new model is highest, and is approximately 3%, 12% and 26% during mild, moderate and severe vapor channeling, respectively.

4. Conclusions

The mathematical formulation of a new model through refinement of the existing RTD approach has been presented in this work. This new model has been validated for the ideal flow situations on a tray. In this model, the geometrical partitioning of a tray into compartments allows accounting for the effects of fluid dynamics at intermediate tray locations as well as non-uniform vapor distribution on the tray efficiency. This is successfully demonstrated through analysis of two separate case studies. The influence of flow path length of liquid on the tray efficiency can also be analyzed using similar procedure as followed in the first case study. Further, the literature on stimulus-response experiments lacks the description of RTD function at different tray locations along the liquid flow path, which is imperative for the application and validation of this model. Thus, only theoretical development on this model has been shown here. An in-house facility has been constructed at HZDR for RTD studies on an 800 mm. diameter sieve tray. The experiments are currently being performed on this facility, which would allow the experimental validation of this model in the future. The proposed development is also beneficial towards realizing a hybrid methodology, i.e. using tray efficiency models supplemented with fluid dynamics information from validated CFD models, for efficiency predictions in the future.

Nomenclature

L	-	Liquid flow rate (kmol/s)	m	-	Slope of the VLE line (-)
t	-	Time (s)	V	-	Vapor flow rate (kmol/s)
W	-	Weir length (m)	w	-	Direction $\perp$ to the bulk liquid flow direction (-)
Z_1	-	Flow path length (m)	z	-	Bulk liquid flow direction (-)
λ	-	Stripping factor $(= mV/L)$ (-)	$\otimes$	-	Convolution integral

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