 

# A MODIFIED MODEL OF COMPUTATIONAL MASS TRANSFER FOR DISTILLATION COLUMN

Z. M. Sun, X. G. Yuan*, C. J. Liu, K. T. Yu
State Key Laboratory for Chemical Engineering (Tianjin University) and
School of Chemical Engineering and Technology, Tianjin University,
Tianjin 300072, People's Republic of China

The Computational Mass Transfer (CMT) model is composed of the basic differential mass transfer equation, closed by auxiliary equations and the appropriate accompanying CFD formulation. In the present modified CMT model, the closing auxiliary equations in the $\overline{c^2} - \varepsilon_c$ model given by Liu (2003) are further simplified for reducing the computational complication. By this model, the turbulent mass transfer diffusivity, the three-dimensional velocity/concentration profiles can be predicted simultaneously. To demonstrate the feasibility of the simplified CMT model, simulation was made for distillation column, and the results are compared with the experimental data taken from literatures. In applying the modified model to the simulation of a commercial scale distillation tray column, the predictions of the concentration at the outlet of each tray and the tray efficiency are satisfactorily confirmed by the published experimental data.

KEYWORDS: Computational Mass Transfer (CMT), $\overline{c^2} - \varepsilon_c$ model, turbulent mass transfer diffusivity, simulation, sieve tray column

## INTRODUCTION

Distillation is the most widely used industrial separation technique due to its reliability in large-size column application and its maturity in engineering practice. However, the estimation of distillation tray efficiency has long been relying on experience, the design of distillation columns is essentially empirical in nature (Zuiderweg, 1982; Lockett, 1986), due to the lack of in-depth understanding of the processes occurring inside a distillation column. With the development of computer technology, it becomes possible to investigate the transfer processes numerically. The Computational Fluid Dynamics (CFD) has been used successfully in the field of chemical engineering as such a tool, and attempts have been made by a number of authors (Yu, 1992; Zhang and Yu, 1994; Wang et al., 2004; Krishna et al., 1999; van Baten and Krishna, 2000; Gesit et al., 2003 etc.) in the simulation of distillation process and equipment.

The idea of using CFD to incorporating the prediction on tray efficiency relies on the fact that the hydrodynamics is an essential influential factor for mass transfer in both the interface and bulk flow. This in fact opens an issue on the computation for mass transfer prediction based on the fluid dynamics computation. This was defined as Computational Mass Transfer (CMT) by Liu (2003), who proposed a two-equation model with a

*Corresponding author. Tel.: +86 22 27404732, Fax: +86 22 27404496, E-mail: yuanxg@tju.edu.cn

concentration variance $\overline{c^2}$ equation and its dissipation rate $\varepsilon_c$ equation as a measure to the closure of the differential mass transfer equation. The CMT model by Liu has been applied successfully to predict the turbulent mass transfer diffusivity and efficiency of a commercial scaled distillation column by Sun et al. (2005). However, Liu's model is of proto type as its initial form is complicated and the computation is tedious. In the present paper, the $\overline{c^2} - \varepsilon_c$ model of Liu (2003) is simplified and the model constants are ascertained. The computed results are then compared with the experimental data taken from literatures to demonstrate the reliability of the CMT model.

## PROPOSED MODEL FOR COMPUTATIONAL MASS TRANSFER

### SIMPLIFICATION OF $\overline{c^2} - \varepsilon_c$ MODEL

The instantaneous equation of turbulent mass transfer can be written as follows:

$$\frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} = D \frac{\partial^2 C}{\partial x_j^2} + S_C \tag{1}$$

where $U$ and $C$ are the instantaneous velocity and concentration respectively. In the model developed by Liu (2003), this equation, with Boussinesq's assumption, was given in a Reynolds average form:

$$\frac{\partial \overline{C}}{\partial t} + \overline{U}_j \frac{\partial \overline{C}}{\partial x_j} = \frac{\partial}{\partial x_j}\left( D \frac{\partial \overline{C}}{\partial x_j} - \overline{u_j c} \right) + S_C \tag{2}$$

According to Liu (2003), the turbulent mass flux $\overline{u_j c}$ in equation (2) can be expressed in terms of turbulent mass transfer diffusivity $D_t$ and concentration gradient, adopting the assumptions of Colin and Benkenida (2003):

$$-\overline{u_j c} = D_t \frac{\partial \overline{C}}{\partial x_j} \tag{3}$$

with

$$D_t = C_t k \left( \frac{k}{\varepsilon} \frac{\overline{c^2}}{\varepsilon_c} \right)^{1/2} \tag{4}$$

In equation (4), $\overline{c^2}$ is the concentration variance and $\varepsilon_c$ is the dissipation rate of concentration variance. A CMT model, named as $\overline{c^2} - \varepsilon_c$ model was developed by Liu (2003) by deducing the following auxiliary equations for $\overline{c^2}$ and $\varepsilon_c$, to achieve closure of the

mass transfer equation (2) combined with CFD model equations.

$$\overline{c^2} \text{ equation: } \frac{\partial \overline{c^2}}{\partial t} + \overline{U}_j \frac{\partial \overline{c^2}}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(D + \frac{D_t}{\sigma_c}\right)\frac{\partial \overline{c^2}}{\partial x_j}\right] - 2\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j} - 2\varepsilon_c \tag{5}$$

$$\varepsilon_c \text{ equation: } \frac{\partial \varepsilon_c}{\partial t} + \overline{U}_j \frac{\partial \varepsilon_c}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(D + \frac{D_t}{\sigma_{\varepsilon_c}}\right)\frac{\partial \varepsilon_c}{\partial \overline{c^2}}\right] - C_{c1}\frac{\varepsilon_c}{\overline{c^2}}\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j} - C_{c2}\frac{\varepsilon_c^2}{\overline{c^2}} - C_{c3}\overline{u_i u_j}\frac{\partial \overline{U}_i}{\partial x_j}\frac{\varepsilon_c}{k} - C_{c4}\frac{\varepsilon \varepsilon_c}{k} + \gamma D_t \frac{\partial^2 \overline{C}}{\partial x_j \partial x_k} \tag{6}$$

where the constants are: $C_t = 0.11$, $C_{c1} = 1.8$, $C_{c2} = 2.2$, $C_{c3} = 0.72$, $C_{c4} = 0.8$, $\sigma_c = 1.0$, $\sigma_{\varepsilon_c} = 1.0$. Hereinafter, the model with the auxiliary equation given by equation (5) and equation (6) is referred to as *original model*.

It could be found that, the computing tediousness comes mainly from the source terms in $\varepsilon_c$ equation, in which not only differential but also algebraic terms of variables are included. In fact this could be simplified in the course of deduction of the $\varepsilon_c$ equation. Taking the derivative of the equation (1) with respect to $x_k$ and multiplying by $2D\partial c/\partial x_k$ and averaging, the $\varepsilon_c$ equation is given as below:

$$\frac{\partial \varepsilon_c}{\partial t} + \overline{U}_j \frac{\partial \varepsilon_c}{\partial x_j} = \frac{\partial}{\partial x_j}\left[D\frac{\partial \varepsilon_c}{\partial x_j} - \overline{u_j \varepsilon_c}\right] - 2D\overline{\frac{\partial c}{\partial x_j}\frac{\partial u_k}{\partial x_j}}\frac{\partial \overline{C}}{\partial x_k} - 2D\overline{u_j}\overline{\frac{\partial c}{\partial x_k}}\frac{\partial^2 \overline{C}}{\partial x_j \partial x_k} - 2D\overline{\frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_j}}\frac{\partial \overline{U}_j}{\partial x_k} - 2D\overline{\frac{\partial c}{\partial x_j}\frac{\partial u_j}{\partial x_k}\frac{\partial c}{\partial x_k}} - 2D^2\overline{\frac{\partial^2 c}{\partial x_j \partial x_k}\frac{\partial^2 c}{\partial x_j \partial x_k}} \tag{7}$$

Applying the treatment similar to the Reynolds stress, the turbulent diffusion term $\overline{u_j \varepsilon_c}$ can be expressed by the following gradient type equation:

$$-\overline{u_j \varepsilon_c} = \left(D_t/\sigma_{\varepsilon_c}\right)\partial \varepsilon_c/\partial x_j \tag{8}$$

Here we define the second, third and fourth terms on the right hand side of equation (7) as the production part:

$$P_{\varepsilon_c} = -2D\overline{\frac{\partial c}{\partial x_j}\frac{\partial u_k}{\partial x_j}}\frac{\partial \overline{C}}{\partial x_k} - 2D\overline{u_j}\overline{\frac{\partial c}{\partial x_k}}\frac{\partial^2 \overline{C}}{\partial x_j \partial x_k} - 2D\overline{\frac{\partial c}{\partial x_k}\frac{\partial c}{\partial x_j}}\frac{\partial \overline{U}_j}{\partial x_k} \tag{9}$$

and the following two terms on the right hand side of equation (7) as the dissipation part:

$$\Sigma_{\varepsilon_c} = -2D\overline{\frac{\partial c}{\partial x_j}\frac{\partial u_j}{\partial x_k}\frac{\partial c}{\partial x_k}} - 2D^2\overline{\frac{\partial^2 c}{\partial x_j \partial x_k}\frac{\partial^2 c}{\partial x_j \partial x_k}} \tag{10}$$

The simplification of the $\varepsilon_c$ equation might resemble the treatment of $\varepsilon$ equation in the conventional CFD model. The modeling of the production part of $\varepsilon$ equation in CFD by Zhang (2002) is given by:

$$\textit{production part of } \varepsilon \textit{ equation} = C_{\varepsilon 1}\frac{1}{\tau} \times \textit{production part of } k \textit{ equation} \tag{11}$$

where $\tau$ is the time scale and can be expressed as $k/\varepsilon$ in CFD.

With the same principle, the production part of $\varepsilon_c$ equation can be modeled as:

$$\textit{production part of } \varepsilon_c \textit{ equation} = C_{c1}\frac{1}{\tau} \times \textit{production part of } \overline{c^2} \textit{ equation} \tag{12}$$

where the concentration time scale $\overline{c^2}/\varepsilon_c$ is used to replace $\tau$. The production part of $\overline{c^2}$ equation is $\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j}$, then the final form of the production part of $\varepsilon_c$ equation can be written as:

$$P_{\varepsilon_c} = -C_{c1}\frac{\varepsilon_c}{\overline{c^2}}\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j} \tag{13}$$

Similarly, comparing with the dissipation part of $\varepsilon$ equation in CFD, the dissipation part of $\varepsilon_c$ equation can be modeled as:

$$\textit{dissipation part of } \varepsilon_c \textit{ equation} = C_{c2}\frac{1}{\tau} \times \textit{dissipation part of } \overline{c^2} \textit{ equation} \tag{14}$$

Since the dissipation part of $\overline{c^2}$ equation is $\varepsilon_c$, then, with $\overline{c^2}/\varepsilon_c$ replacing $\tau$ again, equation (10) becomes:

$$\Sigma_{\varepsilon_t} = -C_{c2}\frac{\varepsilon_c^2}{\overline{c^2}} - C_{c3}\frac{\varepsilon\varepsilon_c}{k} \tag{15}$$

The $\varepsilon_c$ equation becomes finally:

$$\frac{\partial \varepsilon_c}{\partial t} + \overline{U}_j\frac{\partial \varepsilon_c}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(D + \frac{D_t}{\sigma_{\varepsilon_c}}\right)\frac{\partial \varepsilon_c}{\partial x_j}\right] - C_{c1}\frac{\varepsilon_c}{\overline{c^2}}\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j} - C_{c2}\frac{\varepsilon_c^2}{\overline{c^2}} - C_{c3}\frac{\varepsilon\varepsilon_c}{k} \tag{16}$$

The value of $C_t$ in equation (4) was defined as $C_t = C_\mu/Sc_t\sqrt{R}$, where $C_\mu$ is the coefficient in the CFD modeling equation $\nu_t = C_\mu k^2/\varepsilon$, which is adopted generally to

be 0.09. In considering the turbulent Schmidt number $Sc_t = \nu_t/D_t = 0.7$ and the time scale ratio $R = \tau_c/\tau_u = \left(\overline{c^2}/\varepsilon_c\right)/(k/\varepsilon) = 0.9$ (Lemoine et al., 2000), we obtain $C_t = 0.14$. According to the Colin and Benkenida (2003), we choose $C_{c1}$ to be 2.0. Similar to the treatment of Nagano and Kim (1988), the constants $C_{c2}$ and $C_{c3}$ are given as $C_{c2} = R(C_{\varepsilon 2} - 1)$ and $C_{c3} = 2/R$ respectively with $C_{s2} = 1.92$, which is taken from standard $k - \varepsilon$ model (equation (24) and equation (25)). Consequently, the constants in the present model are as: $C_t = 0.14$, $C_{c1} = 2.0$, $C_{c2} = 0.83$, $C_{c3} = 2.22$, $\sigma_c = 1.0$, $\sigma_{\varepsilon_c} = 1.0$.

In fact, by comparing $C_{c2}$ and $C_{c3}$ and considering the value of time scale ratio $R$, the term of $C_{c3}\varepsilon\varepsilon_c/k$ is about 3 times of $C_{c2}\varepsilon_c^2/\overline{c^2}$ and the latter may be neglected without affecting too much the result as shown in the subsequent section. Then the $\varepsilon_c$ equation could be further simplified as:

$$\frac{\partial \varepsilon_c}{\partial t} + \overline{U}_j \frac{\partial \varepsilon_c}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(D + \frac{D_t}{\sigma_{\varepsilon_c}}\right)\frac{\partial \varepsilon_c}{\partial x_j}\right] - C_{c1}\frac{\varepsilon_c}{\overline{c^2}}\overline{u_j c}\frac{\partial \overline{C}}{\partial x_j} - C_{c3}\frac{\varepsilon\varepsilon_c}{k} \tag{17}$$

Hereinafter, the model with equation (16) is referred to as Model I, and that with equation (17) as Model II.

## APPLICATION OF THE PROPOSED CMT MODEL TO DISTILLATION COLUMN SIMULATION

### CFD equations

To simulate the velocity profile on distillation tray, the equations of the steady-state continuity and momentum for the liquid phase in two-phase flow are adopted. In the present model, the liquid volume fraction is considered and the interaction between the vapor and liquid phases is attributed to the source term and is also implicitly involved in the velocity of the liquid phase. The model can be written as:

$$\frac{\partial \alpha_L \overline{U}_i}{\partial x_i} = 0 \tag{18}$$

$$\frac{\partial \alpha_L \overline{U}_j \overline{U}_j}{\partial x_j} = -\alpha_L \frac{1}{\rho_L}\frac{\partial \bar{p}}{\partial x_i} + \alpha_L g + \frac{\partial}{\partial x_j}\left[\alpha_L \nu \frac{\partial \overline{U}_i}{\partial x_j} - \alpha_L \overline{u_i u_j}\right] + S_{Mi} \tag{19}$$

where $S_{Mi}$ is the source term representing the momentum exchange between vapor and liquid phases; and by applying the Boussinisque's relation:

$$-\overline{u_i u_j} = \nu_t\left(\frac{\partial \overline{U}_i}{\partial x_j} + \frac{\partial \overline{U}_j}{\partial x_i}\right) - \frac{2}{3}\delta_{ij}k \tag{20}$$

We assume that the liquid volume fraction $\alpha_L$ is not varying with the position, and given by the correlation of Bennett et al. (1983):

$$\alpha_L = \exp\left[-12.55\left(U_s\sqrt{\frac{\rho_G}{\rho_L-\rho_G}}\right)^{0.91}\right] \tag{21}$$

For the source term in equation (19), the drag force is usually employed to interpret the interaction between individual bubble and liquid, as did by Krishna et al. (1999), Gesit et al. (2003) and Wang et al. (2004). Liu et al. (2000) gave a fairly good prediction for a two-dimensional and two-phase flow on distillation tray with only considering the body force given previously by Zhang et al. (1994). Such considerations are adopted in the present work for the source term:
in the $x$ and $y$ coordinates:

$$S_{Mi} = -\frac{\rho_G U_s}{\rho_L h_f} U_i \quad (i = x, y) \tag{22}$$

in the $z$ coordinate (Krish et al., 1999)

$$S_{Mz} = \frac{(1-\alpha_L)^3}{U_s^2} g(\rho_L-\rho_G)\left|\vec{U}_G - \vec{U}_L\right|(U_s - U_{Lz}) \tag{23}$$

where the froth height is estimated by the correlation $h_f = h_l/\alpha_L$, in which the clear liquid height $h_l$ is calculated by the AIChE correlation (1958): $h_l = 0.0419 + 0.189\,h_w - 0.0135F_s + 2.45q_{L/lw}$.

In closing equation (19), the following standard $k$–$\varepsilon$ method is used.

$$\frac{\partial k}{\partial t} + \overline{U}_j\frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] - \overline{u_i u_j}\frac{\partial \overline{U}_i}{\partial x_j} - \varepsilon \tag{24}$$

$$\frac{\partial \varepsilon}{\partial t} + \overline{U}_j\frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j}\left[\left(\nu + \frac{\nu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] - C_{\varepsilon 1}\frac{\varepsilon}{k}\overline{u_i u_j}\frac{\partial \overline{U}_i}{\partial x_j} - C_{\varepsilon 2}\frac{\varepsilon^2}{k} \tag{25}$$

The model parameters are customary chosen to be $C_\mu = 0.09$, $C_1 = 1.44$, $C_2 = 1.92$, $\sigma_k = 1.0$, $\sigma_\varepsilon = 1.3$.

Mass transfer equation
The equation governing concentration profile of distillation tray is:

$$\frac{\partial \alpha_L \overline{U}_j \overline{C}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\alpha_L D\frac{\partial \overline{C}}{\partial x_j} - \alpha_L \overline{u_j c}\right) + S_C \tag{26}$$

where $S_c$ is the source term for mass transfer between vapor and liquid phases: $S_C = k_L a\left(\overline{C^*} - \overline{C}\right)$ with $k_L$ as the liquid-phase mass transfer coefficient and $a$ as the

effective vapor-liquid interfacial area. The correlation for $k_La$ given by Zuiderweg (1982) was used. The steady form of equations (4), (5) and (16) (or equation (17)) are used to close equation (26).

Boundary conditions

The inlet conditions of $\overline{U} = \overline{U}_{in}$, $\overline{C} = \overline{C_{in}}$ are taken and that for the $k-\varepsilon$ equations takes the conventional formulas (Nallasamy, 1987): $k_{in} = 0.003\overline{U}^2_{xin}$ and $\varepsilon_{in} = 0.09\,k_{in}^{3/2}/(0.015 \times W)$. The inlet conditions of $\overline{c^2} - \varepsilon_c$ equations given by Liu (2003) and Sun et al. (2005) are used: $\overline{c^2}_{in} = \left(0.082 \cdot (\overline{C^*} - \overline{C_{in}})\right)^2$ and $\varepsilon_{cin} = R(\varepsilon_{in}/k_{in})\overline{c^2}_{in}$. At the outlet, we have $p = 0$, and $\partial\overline{C}/\partial x = 0$. The boundary conditions at the tray floor, the outlet weir and the column wall are considered as non-slip, and the conventional logarithm law expression is employed. At the interface of the vapor and liquid, all the stresses are equal to zero: $\partial u_x/\partial z = 0$, $\partial u_y/\partial z = 0$, and $u_z = 0$. Similarly, both at the wall and the interface, the concentration flux is equal to zero.

## COMPUTATIONAL RESULT OF CMT MODEL FOR DISTILLATION COLUMN

### CONCENTRATION DISTRIBUTION

A commercial scale sieve tray column for distillation reported by Sakata and Yanagi (1979) is simulated. The feed is a mixture of cyclohexane-n-heptane and the operating pressure is 165 kPa. Detailed data about the column are available in Sakata and Yanagi (1979). The liquid in the downcomer is assumed to be completely mixed and the computation followed a tray-by-tray scheme to simulate the tray cascade.

As a sample of the computed results, Figure 1 shows the computed concentration distribution on tray 8. It can be seen that the concentration profiles computed by the three different models are similar. Unfortunately, no experimental data on the concentration field of a tray is available at the present in the literature for the comparison. However, we may compare indirectly by means of the outlet concentration of each tray. From Figure 2 it can be seen that the computed outlet concentration of each tray is in good agreement with the experimental measurement except for the tray 4. As we understand from both theory and experiment for the total reflux operation, the plot of outlet

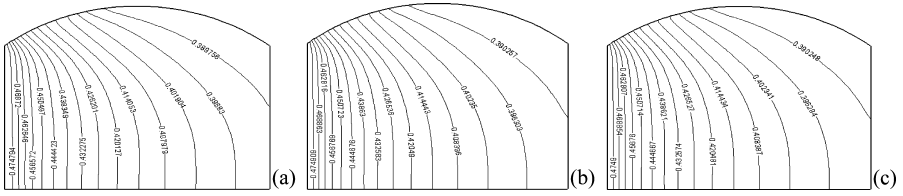


**Figure 1.** Concentration profile of x–y plane on tray 8 at 20 mm above the floor (a) Original Model, (b) Model I, (c) Model II

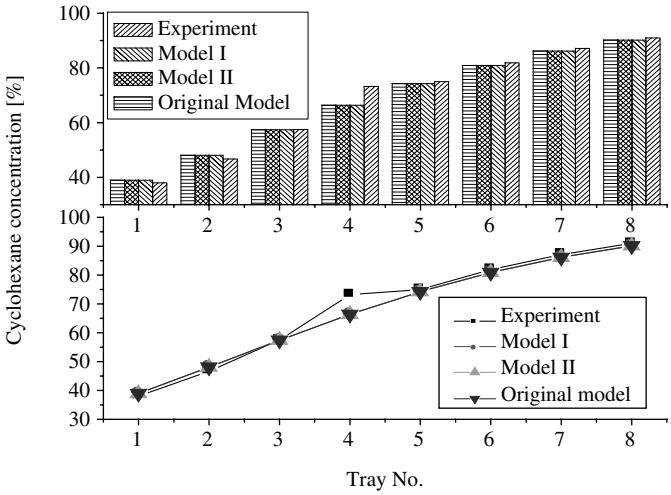


**Figure 2.** Predicted concentration vs. experimental measurement

concentration of all trays should be approximately forming a smooth curve under normal performance. The deviation on tray 4 is likely to be due to experimental error or some other unknown reasons.

The Murphree efficiency for each tray is also compared with experimental data as shown in Figure 3. Except for tray 4 and 3, the predicted results are in agreement with the measurement. The overall tray efficiency can be evaluated by the Fenske-Underwood equation. The predicted overall tray efficiency is 88.26% by Original Model, 88.25% by Model I and 88.25% by Model II, while the experimental measurement is 89.4%.

## TURBULENT MASS TRANSFER DIFFUSIVITY DISTRIBUTION

As a result of the present CMT simulation, Figure 4 gives the turbulent mass transfer diffusivity profiles on tray 1 for the same column predicted by Model II. It can be seen from the figures that $D_t$ is quite diverse. If we take the volume average value of $D_t$, the order of magnitude is about $10^{-2}$–$10^{-3}$, which is close to those reported in the literatures (Yu et al., 1990; Cai and Chen, 2004). Figure 5 gives the comparison of the volume average values of $D_t$ computed by Model I and Model II with the average experimental data for commercial scaled column reported by Cai and Chen (2004). It demonstrates that the simplified model can give results agree well with the experiments.

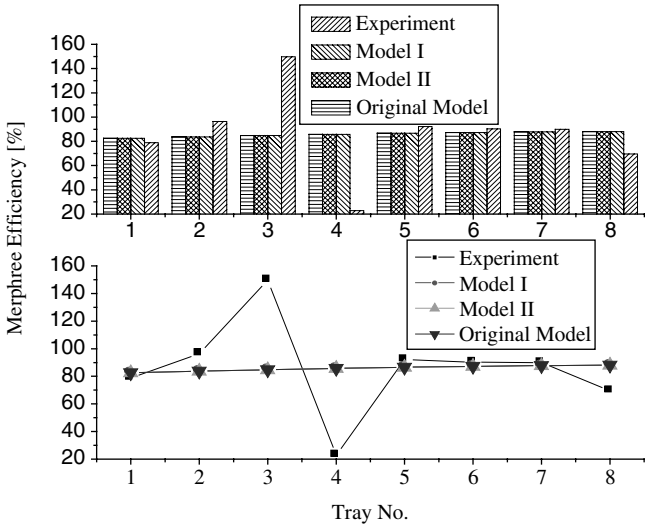


**Figure 3.** Predicted tray efficiency $E_{MV}$ vs. experimental measurement

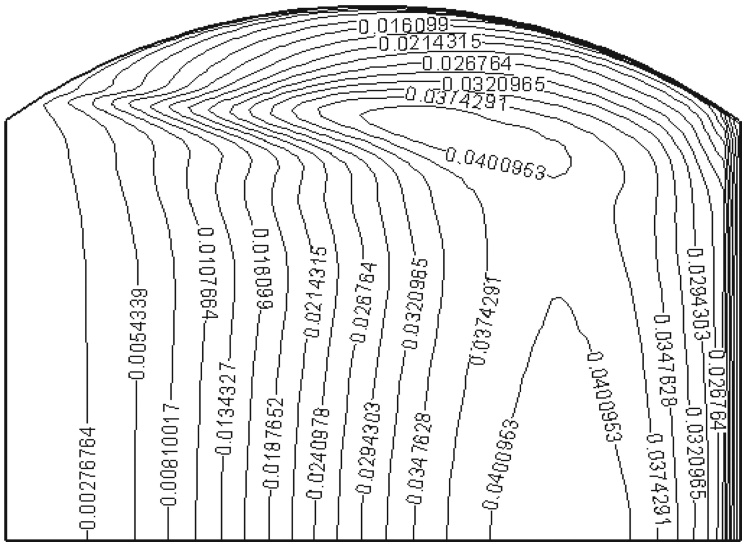


**Figure 4.** Turbulent mass transfer diffusivity profile at 20 mm above the floor (Model II)

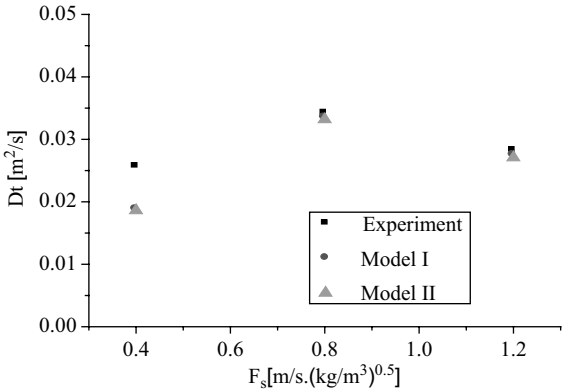


**Figure 5.** Experimental vs. computational of turbulent mass transfer diffusivity

## CONCLUSION

The $\overline{c^2} - \varepsilon_c$ model of Liu (2003) is simplified and the model constants are ascertained. The proposed simplified CMT model is applied to distillation column simulation and the results are compared with the experimental data by Sakata and Yanagi (1979). The comparison reveal that the simplified models can give good predictions on the turbulent mass transfer diffusivity, while the computed concentrations at the outlet of each tray and the tray efficiency by these two models are all in satisfactory agreement with the published experimental data. The simplified computational mass transfer model has shown to be a effective tool to predict the turbulent mass transfer diffusivity, concentration profile on a tray as well as the tray efficiency of a distillation column.

## ACKNOWLEDGEMENT

The authors wish to acknowledge the financial support by National Natural Science Foundation of China (No. 20136010), and the assistance by the staffs in the State Key Laboratories of Chemical Engineering (Tianjin University).

## NOTATION

| | |
|---|---|
| $a$ | specific vapor-liquid contacting area, $m^2 \cdot m^{-3}$ |
| $C_t$, $C_{c1}$, $C_{c2}$, $C_{c3}$ | turbulence model constants for the concentration field |
| $C_\mu$, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$ | turbulence model constants for the velocity field |
| $C$ | instantaneous concentration (mass fraction) |
| $\bar{C}$ | time average concentration (mass fraction) |
| $c$ | fluctuating concentration (mass fraction) |

| | |
|---|---|
| $\overline{c^2}$ | concentration variance |
| $D$ | molecular mass transfer diffusivity, $m^2 \cdot s^{-1}$ |
| $D_t$ | turbulent mass transfer diffusivity, $m^2 \cdot s^{-1}$ |
| $F_s$ | F-factor ($F_s = u_s \sqrt{\rho_G}$) |
| $h_f$ | froth height, m |
| $h_l$ | clear liquid height, m |
| $k$ | turbulent kinetic energy, $m^2 \cdot s^{-2}$ |
| $k_L$ | liquid mass transfer coefficient, $m \cdot s^{-1}$ |
| $R$ | time-scale ratio |
| $Re$ | Reynolds Number |
| $S_C$ | source of inter phase mass transfer |
| $S_{\mathrm{Mi}}$ | source of inter phase momentum transfer |
| $t$ | time, s |
| $U$ | instantaneous velocity, $m \cdot s^{-1}$ |
| $\overline{U}$ | time average velocity, $m \cdot s^{-1}$ |
| $U_{\mathrm{s}}$ | superficial vapor velocity, $m \cdot s^{-1}$ |
| $u$ | fluctuating velocity, $m \cdot s^{-1}$ |

GREEK LETTERS

| | |
|---|---|
| $\alpha_L$ | liquid volume fraction |
| $\varepsilon$ | turbulent dissipation, $m^2 \cdot s^{-3}$ |
| $\varepsilon_c$ | dissipation rate of $\overline{c^2}$, $s^{-1}$ |
| $v_t$ | turbulent viscosity, $m^2 \cdot s^{-1}$ |
| $\rho$ | density, $kg \cdot m^{-3}$ |
| $\sigma_c$, $\sigma_\varepsilon$, $\sigma_k$ | turbulence model constants for diffusion of $\overline{c^2}$, $\varepsilon$, $k$ |
| $\tau$ | time scale, s |

SUBSCRIPTS

| | |
|---|---|
| *i, j, k* | x, y, and z coordinates |
| *x, y, z* | coordinates |

## REFERENCES

AIChE Research Committee, (1958). Bubble tray design manual. AIChE, New York.

Bennett, D.L., Rakesh, A., Cook, P.J., (1983). New pressure drop correlation for sieve tray distillation columns. AIChE Journal., 29, 434–442.

Cai, T.J., Chen, G.X., (2004). Liquid back-mixing on distillation trays. Ind. Eng. Chem. Res., 43, 2590–2597.

Colin, O., Benkenida, A., (2003). A new scalar fluctuation model to predict mixing in evaporating two-phase flows. Combustion and Flame, 134, 207–227.

Gesit, G., Nandakumar, K., Chuang, K.T., (2003). CFD Modeling of flow patterns and hydraulics of commercial-scale sieve trays. AIChE Journal, 49, 910–924.

Krishna, R., van Baten, J.M., Ellenberger, J., Higler, A.P., Taylor, R., (1999). CFD simulations of sieve tray hydrodynamics. Chemical Engineering Research and Design, Trans IChemE, Part A., 77, 639–646.

Lemoine, F., Antoine, Y., Wolff, M., Lebouche, M., (2000). Some experimental investigations on the concentration variance and its dissipation rate in a grid generated turbulent flow. International J. Heat and Mass Transfer, 43, 1187–1199.

Liu, B.T., (2003). Study of a new mass transfer model of CFD and its application on distillation tray. Ph.D. Dissertation, Tianjin University, Tianjin, China.

Liu, C.J., Yuan, X.G., Yu, K.T., Zhu, X.J., (2000). A Fluid-dynamics Model for flow pattern on a distillation tray. Chem. Eng. Sci., 55, 2287–2294.

Lockett, M.J., (1986). Distillation Tray Fundamentals. Cambridge University Press, Cambridge.

Nagano, Y., Kim, C., (1988). A two-equation model for heat transport in wall turbulent shear flows. J. Heat Transfer, Transactions ASME, 110, 583–589.

Nallasamy, M., (1987). Turbulence models and their applications to the prediction of internal flows.; Comp. Fluids, 15, 151–194.

Sakata, M., Yanagi, T., (1979). Performance of a commercial scale sieve tray. IChemE Symposium series, 56, 3.2/21–34.

Sun, Z.M., Liu, B.T., Yuan, X.G., Liu, C.J., Yu, K.T., (2005). New Turbulent Model for Computational Mass Transfer and its application to a commercial-scale distillation column. Ind. Eng. Chem. Res., 44, 4427–4434.

van Baten, J.M., Krishna, R., (2000). Modelling sieve tray hydraulics using computational fluid dynamics. Chemical Engineering Journal, 77, 143–151.

Wang, X.L., Liu, C.J., Yuan, X.G., Yu, K.T., (2004). Computational fluid dynamics simulation of three-dimensional liquid flow and mass transfer on distillation column trays. Ind. Eng. Chem. Res., 43, 2556–2567.

Yu, K.T., (1992). Some progress of distillation research and industrial applications in China. IChemE Symposium Series, v 1: A139–A166.

Yu, K.T., Huang, J., Li, J.L., Song, H.H., (1990). Two-dimensional flow and eddy diffusion on a sieve tray. Chem. Eng. Sci., 45, 2901–2906.

Zhang, M.Q., Yu, K.T., (1994). Simulation of two dimensional liquid phase flow on a distillation tray. Chinese J. Chemical Engineering, 2, 63–71.

Zhang, Z.Sh., (2002).Turbulence. National Defence Industry Press, Beijing, 258.

Zuiderweg, F.J., (1982). Sieve tray—a view on the state of the art. Chem. Eng. Sci., 37, 1441–1464.