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A modified model of computational mass transfer for distillation column

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Abstract

The computational mass transfer (CMT) model is composed of the basic differential mass transfer equation, closing with auxiliary equations, and the appropriate accompanying CFD formulation. In the present modified CMT model, the closing auxiliary equations $\overline{c^2}$–ε_c [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; 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. Industrial and Engineering Chemistry Research 44, 4427–4434] are further simplified for reducing the complication of computation. At the same time, the CFD formulation is also improved for better velocity field prediction. By this complex model, the turbulent mass transfer diffusivity, the three-dimensional velocity/concentration profiles and the efficiency of mass transfer equipment can be predicted simultaneously. To demonstrate the feasibility of the proposed simplified CMT model, simulation was made for distillation column, and the simulated results are compared with the experimental data taken from literatures. The predicted distribution of liquid velocity on a tray and the average mass transfer diffusivity are in reasonable agreement with the reported experimental measurement [Solari, R.B., Bell, R.L., 1986. Fluid flow patterns and velocity distribution on commercial-scale sieve trays. AI.Ch.E. Journal 32, 640–649; Cai, T.J., Chen, G.X., 2004. Liquid back-mixing on distillation trays. Industrial and Engineering Chemistry Research 43, 2590–2597]. In applying the modified model to 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 [Sakata, M., Yanagi, T., 1979. Performance of a commercial scale sieve tray. Institution of Chemical Engineers Symposium Series, vol. 56, pp. 3.2/21–3.2/34]. Furthermore, the validity of the present model is also shown by checking the computed results with a reported pilot-scale tray column [Garcia, J.A., Fair, J.R., 2000. A fundamental model for the prediction of distillation sieve tray efficiency. 1. Database development. Industrial and Engineering Chemistry Research 39, 1809–1817] in the bottom concentration and the overall tray efficiency under different operating conditions. The modified CMT model is expected to be useful in the design and analysis of distillation column.

Keywords: Computational mass transfer (CMT); $\overline{c^2}$–ε_c model; Turbulent mass transfer diffusivity; Simulation; Sieve tray

1. Introduction

Distillation, the most commonly used separation process for the liquid mixture, has been widely used in the chemical and allied industries due to its reliability in large-size column application and its maturity in engineering practice. Among the distillation equipments, the tray column is popularly employed in the industrial production for its simple structure and low cost of investment. However, the estimation of distillation tray efficiency, which might vary significantly from one to another and is extremely influential to the technical–economical behaviors of a column, has long been relying on experience, and the design of distillation columns is essentially empirical in nature (Zuiderweg, 1982; Lockett, 1986). The lack of in-depth understanding of the processes occurring inside a distillation column is known to be the major barrier to the proper estimation and improvement of the column performance (AIChE, 1998).

With the development of computer technology and the advancement in numerical methods, it becomes possible to investigate the transfer process numerically with the chemical engineering and cross-disciplinary theories. The numerical

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approaches have many advantages, such as offering more in-depth information than that upon experiments, shortening the cycles for process and equipment development by visualizing and comparing the results of virtual trials and modifications. The computational fluid dynamics (CFD) has been used successfully in the field of chemical engineering as a tool.

In the simulation of distillation process and equipment, Yu (1992) and Zhang and Yu (1994) presented a two-dimensional CFD model for simulating the liquid phase flow on a sieve tray, in which the k–ε equations were employed to achieve the closure of the equation system and a body force of vapor was included in the source term of the momentum equation to consider the interacting effect of vapor and liquid phases. On this basis, Liu et al. (2000) developed a model describing the liquid-phase flow on a sieve tray with consideration of both the resistance and the bubbling effect generated by the uprising vapor. Later on, Wang et al. (2004) further developed a three-dimensional model considering the effect of vapor by adding drag force, lift force, virtual mass force and body force in the model, and simulated a 1.2-m-diameter column with 10 sieve trays under total reflux. The CFD application to distillation was also made by Krishna et al. (1999) and van Baten and Krishna (2000). They used fully three-dimensional transient simulations to describe the hydrodynamics of trays, and gave liquid volume fraction, velocity distribution and clear liquid height for a rectangular tray and a circular tray, respectively, via a two-phase flow transient model. Also, Fischer and Quarini (1998) proposed a three-dimensional heterogeneous model for simulating tray hydraulics. Mehta et al. (1998) and Gesit et al. (2003) predicted liquid velocity distribution, clear liquid height, froth height, and liquid volume fraction on trays using CFD techniques.

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 interfacial and bulk diffusions, which could be understood by the effect of velocity distribution on concentration profile. This in fact opens an issue on the computation for mass transfer prediction based on the fluid dynamics computation.

The key problem of this approach is the closure of the differential mass transfer equation, as two unknown variables, the concentration and the turbulent mass transfer diffusivity, being involved in one equation. The turbulent mass transfer diffusivity depends not only on the fluid dynamic properties (e.g. turbulence viscosity of the fluid) but also on the fluctuation of concentration in turbulent flow. Liu (2003) proposed a two-equation model with a concentration variance $\overline{c^2}$ equation and its dissipation rate ε_c equation as a measure to the closure of the differential mass transfer equation. Liu's computational mass transfer (CMT) model 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 prototype as its initial form is complicated and the computation is tedious. In the present paper, the $\overline{c^2}$–ε_c model is simplified and the model constants are ascertained. At the same time, the CFD equation is modified in describing the interaction between the vapor and liquid phases to improve the velocity modeling, which is influential to the computed tray efficiency. To testify the validity of the simplification and improvement, the computed results are compared with the experimental data taken from literatures. The agreement between them demonstrates that the modified CMT method can be used effectively in analyzing the performance of existing distillation column as well as assessing the tray efficiency before construction.

2. Proposed model for CMT

2.1. Simplification of $\overline{c^2}$–ε_c model

The instantaneous equation of turbulent mass transfer can be written as follows in the tensor form for avoiding complicated mathematical expression:

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

where U and C are the instantaneous velocity and concentration, respectively. If both U and C are expressed by the time average values $\overline{U}$ and $\overline{C}$, the foregoing equation is transformed to the following Reynolds average form for the transport of average concentration:

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

Similar to Boussinesq's assumption, the turbulent mass flux $\overline{u_j c}$ in Eq. (2) can be expressed in terms of turbulent mass transfer diffusivity D_t and concentration gradient

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

Since the turbulent mass transfer diffusivity D_t is regarded as direct proportional to the product of the characteristic velocity and the characteristic length, we have,

$$D_t = C_t k^{1/2} L_m. \tag{4}$$

With the relationship $L_m = k^{1/2}\tau_m$, $\tau_m = \sqrt{\tau_\mu \tau_c}$, and the definition of two timescales (Colin and Benkenida, 2003) $\tau_\mu = k/\varepsilon$, $\tau_c = \overline{c^2}/\varepsilon_c$, the turbulent mass transfer diffusivity D_t can be written as

$$D_t = C_t k \left(\frac{k}{\varepsilon} \frac{\overline{c^2}}{\varepsilon_c} \right)^{1/2}. \tag{5}$$

In Eq. (5), $\overline{c^2}$ is the concentration variance and ε_c is the dissipation rate of concentration variance, which can be expressed as

$$\varepsilon_c = D \overline{\frac{\partial c}{\partial x_j} \frac{\partial c}{\partial x_j}}. \tag{6}$$

For the closure of the turbulent mass transfer, or the elimination of diffusivity D_t, two auxiliary equations are developed as follows. Substituting $C = \overline{C} + c$ and $U = \overline{U} + u$ into Eq. (1)