# An anisotropic turbulent mass transfer model for simulation of pilot-scale and industrial-scale packed columns for chemical absorption

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## ABSTRACT

An anisotropic turbulent mass transfer model, namely the Reynolds mass flux model (RMF), for simulating the chemical absorption process in packed column is introduced by the use of combined computational methodology. With the present model, the concentration and temperature as well as velocity distributions can be simultaneously obtained. The feature of the proposed model is that the modeled Reynolds mass flux equation is adopted to close the turbulent mass transfer equation so that the Boussinesq's postulation is abandoned and consequently the anisotropy of turbulent mass diffusion can be characterized. The present model is accompanied by the formulations of computational fluid dynamics (CFD) and computational heat transfer (CHT). In mathematical expression of CFD and CHT, the Reynolds stress and Reynolds heat flux equations are used to close the turbulent momentum and heat transfer equations. The simulated results are validated with experimental data for pilot-scale and industrial-scale packed columns and satisfactory agreement is found between them. Furthermore, the Reynolds mass flux and the anisotropic turbulent mass diffusion are characterized and discussed.

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## 1. Introduction

Chemical absorption has been widely used to remove $CO_2$, $H_2S$ and $SO_2$ from flue gas and received much attention nowadays due to the worldwide concern of environmental protection. The accompanied chemical reaction can significantly increase the absorption rate, decrease the amount of absorbent needed and subsequently reduce the size of the absorption column and operating cost.

The mass transfer process in absorption column is strongly coupled with the turbulent flow and the heat effect. Due to the non-uniformly distributed packing porosity [1–3] and the created non-uniformly distributed velocity and temperature as well as concentration, the conventional plug-flow or one dimensional model is not applicable for exploring such complicated mass transfer behavior in absorption column. The use of combined computational methodology, consisting of the recently developed computational mass transfer (CMT) [4] and the established computational heat transfer (CHT) [5,6] as well as computational fluid-dynamics (CFD) enable us to solve this problem with the

rigorous closure of the differential turbulent mass, heat and momentum transfer equations so as to obtain the concentration, temperature and flow profiles in the packed column. And such information is important for a deeper understanding of the transport phenomena in absorption column and also useful in designing a new column or assessing an existing one.

The key to finding the concentration, temperature and velocity profiles in the packed column is to develop a proper method for the closure of the corresponding differential equations. Taking the differential turbulent mass transfer equation at constant density, $\rho$, for example:

$$\frac{\partial(\overline{C})}{\partial t} + \frac{\partial}{\partial x_i}(\overline{U_i C}) = \frac{\partial}{\partial x_i}\left[\left(D\frac{\partial \overline{C}}{\partial x_i} - \overline{u_i' c'}\right)\right] + \overline{S_C} \quad (1)$$

where $\overline{U_i}$ and $\overline{C}$ are respectively the time average velocity and mass concentration (kg m$^{-3}$); $u'$ and $c'$ are respectively the fluctuated velocity and mass concentration; $\overline{S_C}$ represents the source term; $\overline{u_i' c'}$ (kg m$^{-2}$ s$^{-1}$) is an unknown term to be solved, we may called such term as Reynolds mass flux by the similarity with Reynolds stress $-\rho\overline{u_i' u_j'}$ and Reynolds heat flux $-\rho\overline{u_i' T'}$.

The Reynolds mass flux $\overline{u_i' c'}$ is commonly solved by applying the Boussinesq' postulation:

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## Notation

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|---|---|---|---|
| $a$ | packing surface area per unit volume of packed column, $m^{-1}$ | $P^*_{CO_2}$ | partial pressure of $CO_2$ in equilibrium with solutions, kPa |
| $a_e$ | effective area for mass transfer, $m^{-1}$ | $Pr_t$ | turbulent Prandtl number |
| $a_w$ | wetted packing surface area, $m^{-1}$ | $P_t$ | total pressure of gas phase, kPa |
| $\overline{C}$ | average mass concentration of MEA in liquid phase, $kg\ m^{-3}$ | $R$ | radius of the column, m |
| $C_{CO_2}$ | mass concentration of $CO_2$ in the gas phase, kg $CO_2$ per kg carrier gas | $r$ | radial distance from the axis of the column, m |
| $C_{C1}, C_{C2}, C_{C3}$ | parameters in Reynolds mass flux equation | $R_g$ | universal gas constant, $J\ K^{-1}\ mol^{-1}$ |
| $C_{T1}, C_{T2}, C_{T3}$ | parameters in Reynolds heat flux equation | $R_C$ | the rate of reaction, $kmol\ m^{-3}\ s^{-1}$ |
| $C_{u1}, C_{u2}, C_{u3}$ | parameters in Reynolds stress equation | $r_c$ | carbonation ratio ($CO_2$ loading) of the aqueous MEA solutions, mol $CO_2$ per mol MEA |
| $c'$ | fluctuated mass concentration, $kg\ m^{-3}$ | $Re_L$ | Reynolds number of liquid phase base on packing diameter, $Re_L = \rho d_p U_L/h\mu$ |
| $c_p$ | specific heat of liquid phase, $J\ kg^{-1}\ K^{-1}$ | | |
| $D$ | molecular diffusivity, $m^2\ s^{-1}$ | $Re_p$ | Reynolds number of gas phase base on packing diameter, $Re_p = \rho_g d_p U_g/[(\gamma - h)\mu_g]$ |
| $D_t$ | isotropic turbulent mass diffusivity, $m^2\ s^{-1}$ | | |
| $\boldsymbol{D_{t,i}}$ | anisotropic turbulent mass diffusivity, $m^2\ s^{-1}$ | $Sc_t$ | turbulent Schmidt number |
| $E$ | enhancement factor | $\overline{T}$ | average liquid temperature, K |
| $F_{LG}$ | interface drag force between liquid and gas phases, $N\ m^{-3}$ | $T'$ | fluctuated temperature, K |
| | | $U_i$ | superficial velocity of liquid, $m\ s^{-1}$ |
| $F_{LS}$ | flow resistance created by the random packing, $N\ m^{-3}$ | $U_g$ | superficial velocity of gas, $m\ s^{-1}$ |
| $G$ | gas phase flow rate per unit cross-section area, $kg\ m^2\ s^{-1}$ | $\overline{U_i}$ | average interstitial velocity of liquid, $m\ s^{-1}$ |
| | | $U_{slip}$ | slip velocity between gas and liquid phase, $m\ s^{-1}$ |
| $G_c$ | gas flow rate per unit cross-section area of the carrier gas, $kg\ m^2\ s^{-1}$ | $u'_i$ | fluctuated velocity, $m\ s^{-1}$ |
| | | $X$ | molar concentration in liquid phase, $kmol\ m^{-3}$ |
| $g$ | gravitational acceleration, $m\ s^{-2}$ | $x, y$ | axial and radial coordinates |
| $H$ | Henry's constant for $CO_2$ in MEA solutions, $kmol\ m^{-3}\ kPa^{-1}$ | $x_{H_2O}, x_{MEA}$ | molar fraction of water and MEA in aqueous MEA solutions, respectively |
| $H_A$ | physical absorption heat of mol $CO_2$ absorbed, $J\ kmol^{-1}$ | $y_{CO_2}$ | volume fraction of $CO_2$ in gas phase |
| $H_R$ | heat of chemical reaction per mol $CO_2$ absorbed, $J\ kmol^{-1}$ | $z$ | axial position counting from the column bottom, m |
| $K_G$ | overall mass transfer coefficient of gas phase, $kmol\ m^{-2}\ s^{-1}\ kPa^{-1}$ | | |

**Greek symbols**

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|---|---|---|---|
| $k$ | turbulent kinetic energy, $m^2\ s^{-2}$ | $\alpha_t$ | turbulent thermal diffusivity, $m^2\ s^{-1}$ |
| $k_2$ | second-order reaction rate constant, $m^3\ kmol^{-1}\ s^{-1}$ | $\beta$ | volume fraction of liquid phase based on pore space |
| $k_G$ | gas phase mass transfer coefficient, $kmol\ m^{-2}\ s^{-1}\ kPa^{-1}$ | $\chi$ | excess Henry's quantity, $kmol\ m^{-3}\ kPa^{-1}$ |
| $k_L$ | liquid phase mass transfer coefficient, $m\ s^{-1}$ | $\varepsilon$ | turbulent dissipation rate, $m^2\ s^{-3}$ |
| $k_{R,L}$ | liquid phase mass transfer coefficient with chemical reaction, $m\ s^{-1}$ | $\gamma$ | local porosity |
| | | $\gamma_\infty$ | porosity in an unbounded packing |
| $L$ | liquid flow rate per unit cross-section area, $kg\ m^2\ s^{-1}$ | $\mu$ | liquid molecular viscosity, $kg\ m^{-1}\ s^{-1}$ |
| $M$ | quantity of $CO_2$ absorbed by the aqueous solution per unit volume and unit time, $kg\ m^{-3}\ s^{-1}$ | $v_t$ | turbulent kinematic viscosity, $kg\ m^2\ s^{-1}$ |
| | | $\rho, \rho_g$ | liquid and gas density, $kg\ m^{-3}$ |
| $M_{CO_2}, M_{MEA}, M_g$ | molecular weight of $CO_2$, MEA and carrier gas, respectively, $kg\ kmol^{-1}$ | $\sigma$ | surface tension of aqueous solutions, $N\ m^{-1}$ |
| | | $\delta_{ij}$ | Kronecker delta |
| $P_{CO_2}$ | partial pressure of $CO_2$ in main body of gas, kPa | | |

$$-\overline{u'_i c'} = D_t \frac{\partial \overline{C}}{\partial x_i} \qquad (2)$$

It should be mentioned that the term $\overline{u'_i c'}$ is anisotropic as $i = x$, $y, z$ is directional; while the turbulent mass diffusivity $D_t$ is a isotropic coefficient which is applicable to all directions.

The usual way to find the unknown $D_t$ is by using the turbulent Schmidt number model [7,8]. Such model is characterized by $Sc_t = v_t/D_t$, so that $D_t = v_t/Sc_t$. The value of $Sc_t$ can be found either by considering it as a constant ranging from 0.6 to 1.0 [9–11] or expressing it by an empirical correlation obtained from the inert tracer experiment [12]. Nevertheless, the right choice of $Sc_t$ is difficult. The value of $D_t$ found by inert tracer experiment without mass transfer is different from that under mass transfer condition.

To avoid the use of the $Sc_t$ or its experimental expression, a rigorous model, so called $\overline{c'^2} - \varepsilon_{c'}$ model was developed recently [13] and has been successfully applied to predicting a number of mass transfer processes [13–20]. In this model, $D_t$ was calculated by

$D_t = C_{c0} k (\overline{kc'^2}/\varepsilon \varepsilon_{c'})^{1/2}$, where $k, \varepsilon, \overline{c'^2}$ and $\varepsilon_{c'}$ are determined by corresponding model equations. Although the $\overline{c'^2} - \varepsilon_{c'}$ model is an advancement, yet it still retained the postulation of Eq. (2) and the assumption of isotropic diffusivity $D_t$, which is in contradiction with the high anisotropic turbulent diffusion existing in packed columns [21,22]. Li et al. [23] proposed a new model for the simulation of distillation and obtained the concentration field of the packed column by solving the transport equation of Reynolds mass flux $\overline{u'_i c'}$ for the closure of the turbulent mass transfer equation, so that the assumption of isotropic $D_t$ is abandoned. However, for the closure of the accompanied momentum conservation equation, the Boussinesq's postulation is still applied in order to reduce computational effort, and we can call this model as hybrid Reynolds mass flux model (hybrid RMF model). Later, this model was applied to the simulation of chemical absorption process [24]. However, there still remained isotropic implication in modeling the Reynolds stress and Reynolds mass flux equations. Therefore, the hybrid Reynolds mass flux model need be further improved. Recently, the hybrid RMF