Computational fluid dynamics modeling of inter- circulating fluidized bed

WANG Qiang [1,2], MA Peisheng [1], JIA Qingzhu [1,2]*

1. *College of Chemical Engineering, Tianjin University, Tianjin, 300072, China*
2. ** College of Material Science and Chemical Engineering, Tianjin University of Science and Technology, Tianjin, 300222, China,*

Abstract

A new computational fluid dynamics modeling of inter- circulating fluidized bed has been proposed based on the theory of mass transfer and energy transfer as well as momentum transfer. Numerical solution of the model is obtained, and the simulated results are consistent with experiment

Key word: CFD Model; Inter-circulating Fluidized Bed; Mass Transfer; Flux;

Correspondent Address:

Dr WANG Qiang, College of Material Science and Chemical Engineering, Tianjin University of Science and Technology, Tianjin, 300222, China

86-22-60273221 (office); 86-13370356087(mobile); Fax 86-22-23302748;

Email: wang_q@tust.edu.cn

1. INTRODUCTION.

Fluidized bed units are found in many plant operations in chemical, pharmaceutical, environmental protection and mineral industries. Despite their widespread applications, much of the development and design of fluidized bed reactors have been empirical as the complex flow behaviors of gas-liquid flow in these systems makes flow modeling a challenging task [1-3]. The fundamental problem encountered in modeling hydrodynamics of fluidized bed is the motion of the two phases of which the interface is unknown and transient, and the interaction is understood only for a limited range of conditions [4].

Sotudeh-Gharebeagh *et al*.[5] simulated the circulating fluidized bed using ASPEN PLUS based on an isothermal assumption. The kinetic and hydrodynamic subroutines were used for calculating the rates of reactions and predicting the mean axial voidage profile in upper region. The results expressed in terms of mass transfer efficiency. Huilin *et al*.[6] computed a circulating fluidized bed boiler with wide particle size distributions by considering the hydrodynamics, heat transfer and combustion of coal. The models predicted the flue gas temperature, the chemical gas species, and the concentration distributions in reactor.

While most of the previous work focused on circulating fluidized bed[7], the work in our group has been focused on inter-circulating fluidized bed (ICFB). The advantage of ICFB is highly efficient in mass transfer and reaction rate compare with CFB. In this study, the hydrodynamic behavior of a two-dimensional gas-liquid fluidized bed reactor was investigated, and proposed a new computational fluid dynamics modeling of inter-circulating fluidized. CFD simulation results from the model were compared to those obtained by experiments.

2. CFD MODEL of ICFB

We study three-phase flow in porous media under the following assumptions:
(1)one-dimensional flow; (2) gas –liquid flow; (3) isothermal processes; and (4) negligible capillary pressure effects.

So, here the law of conservation of mass could be applied to each species i in mixture, and combined mass flux includes both the molecular flux and the convective flux.

2.1 Conservative of Mass and Momentum for ICFB

$$\frac{\partial \rho_i}{\partial t} = -\nabla \cdot (\rho_i v) - \nabla \cdot j_i + r_i \qquad (1)$$

this is the equation of continuity for species i in a multi-components reacting mixture system. It describes the change in mass concentration of species i with time at affixed point in space by the diffusion and convection of i, as well as by chemical reactions that produce or consume i component. It also can be expressed as follow

$$\frac{D\rho_i}{Dt} = -\rho_i \nabla \cdot v - \nabla \cdot j_i + r_i \qquad (2)$$

$$\rho \frac{Dw_i}{Dt} + w_i \frac{D\rho}{Dt} = -\rho w_i \nabla \cdot v - \nabla \cdot j_i + r_i$$

here

$$\frac{D\rho_i}{Dt} = -\frac{\partial \rho_i}{\partial t} + v \nabla \cdot \rho_i$$

$$v = v_x \delta_x + v_y \delta_y + v_z \delta_z$$

$$\rho_i = \rho w_i$$

$D\rho_i / Dt$ is Lagrange derivation. Both the energy conservative equation and basic equation

$$\rho \frac{D\overline{H}}{Dt} = \rho \frac{D\overline{U}}{Dt} + p(\nabla \cdot \upsilon) + \frac{Dp}{Dt} \qquad (3)$$

$$\rho \frac{D\overline{H}}{Dt} = \rho C_p \frac{DT}{Dt} + \left[\hat{V} - T\left(\frac{\partial \overline{V}}{\partial T} \right)_{p,m_i} \right] \rho \frac{Dp}{Dt} + \sum_{i=1}^{1} \rho \left(\frac{\partial \overline{H}}{\partial m_i} \right)_{T,p,m_j,i \neq j} \frac{Dw_i}{Dt} \qquad (4)$$

$$\frac{\partial}{\partial t}\left[\rho \left(\overline{U} + \frac{1}{2} v^2 \right) \right] = -\nabla \cdot \left[\rho \left(\overline{U} + \frac{1}{2} v^2 \right) \upsilon \right] - \nabla \cdot q - \nabla \cdot (\tau \cdot \nu) + \sum_{i=1}^{n} \rho_i (\nu_i \cdot \phi_i) \qquad (5)$$

then

$$\rho \frac{D}{Dt}\left(\overline{U} + \frac{1}{2} v^2 \right) = -\nabla \cdot q - \nabla \cdot (\tau \cdot \nu) + \sum_{i=1}^{n} \rho_i (\nu_i \cdot \phi_i) \qquad (6)$$

from equation of momentum

$$\frac{\partial (\rho v)}{\partial t} = -\nabla \cdot (\rho v v) - \nabla \cdot \tau + \sum_{i=1}^{n} \rho_i \phi_i \qquad (7)$$

$$\rho \frac{Dv}{Dt} = -\nabla \cdot \tau + \sum_{i=1}^{n} \rho_i \phi_i$$

of thermodynamics for mixture system can be written as

we have

$$\rho\frac{D}{Dt}\left(\frac{1}{2}v^2\right)=-v\cdot(\nabla\cdot\tau)+v\cdot\sum_{i=1}^{n}\rho_i\phi_i=-\nabla\cdot(\tau\cdot v)+\tau^T:\nabla\cdot v+\sum_{i=1}^{n}\rho_i(v\cdot\phi_i) \tag{8}$$

$$\tau^T:\nabla v=p(\nabla\cdot v)-\mu\psi$$

$$\psi=2\left[\left(\frac{\partial v_x}{\partial x}\right)^2+\left(\frac{\partial v_y}{\partial y}\right)^2+\left(\frac{\partial v_z}{\partial z}\right)^2\right]+\left(\frac{\partial v_y}{\partial x}+\frac{\partial v_x}{\partial y}\right)^2+$$

$$+\left(\frac{\partial v_z}{\partial y}+\frac{\partial v_y}{\partial z}\right)^2+\left(\frac{\partial v_x}{\partial z}+\frac{\partial v_z}{\partial x}\right)^2-\frac{2}{3}(\nabla\cdot v)^2$$

$$\rho\frac{D\overline{U}}{Dt}=-\nabla\cdot q-\tau^T:(\nabla v)+\sum_{i=1}^{n}\rho_i(v_i-v)\cdot\phi_i$$

$$\rho_i(v_i-v)=j_i$$

$$\rho\frac{D\overline{U}}{Dt}=-\nabla\cdot q-p(\nabla\cdot v)+\mu\psi+\sum_{i=1}^{n}j_i\cdot\phi_i \tag{9}$$

$$\rho C_p\frac{DT}{Dt}=-\nabla\cdot q+\left(\frac{\partial\ln\overline{V}}{\partial\ln T}\right)_{p,m_i}\frac{Dp}{Dt}+\mu\psi+\sum_{i=1}^{n}j_i\cdot\phi_i+\sum_{i=1}^{n}\frac{\overline{H_i}}{M_i}(\nabla\cdot j_i-r_i) \tag{10}$$

from formula (6) and (8)

take the formula (2) 、（4）、(9) into (3)

Without energy exchanging between the system and surrounding for a isothermal process $\nabla\cdot q=0$, then for system of one-dimensional *x* direction flow

$$\beta T\frac{Dp}{Dt}+\mu\psi+\sum_{i=1}^{n}j_i\cdot\phi_i+\sum_{i=1}^{n}\frac{\overline{H_i}}{M_i}(\nabla\cdot j_i-r_i)=0$$

$$\beta T\frac{\partial p}{\partial t}+\alpha T u_x\frac{\partial p}{\partial x}+\mu\psi+\sum_{i=1}^{n}j_i\cdot\phi_i+\sum_{i=1}^{n}\frac{\overline{H_i}}{M_i}(\nabla\cdot j_i-r_i)=0 \tag{11}$$

$$\beta=\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)$$

so the quasi-linear first order partial differential equation(11), it could be solved from its characteristic line equation

$$\frac{dt}{\beta T}=\frac{dx}{aTu_x}=-\frac{dp}{\mu\psi+\sum_{i=1}^{n}j_i\cdot\phi_i+\sum_{i=1}^{n}\frac{\overline{H_i}}{M_i}(\nabla\cdot j_i-r_i)} \tag{12}$$

2.2 Changing of Pressure in ICFB

The pressure in ICFB could be represented as follow,

$$p = a_1 + b_1 \sin(a_2 + b_2 x)$$

and its boundary conditions

$$x = 0; \qquad p = p_0; \qquad a_2 + b_2 x = \frac{\pi}{2}$$

$$x = L; \qquad p = p_a; \qquad a_2 + b_2 x = \frac{3\pi}{2}$$

then

$$a_2 = \frac{\pi}{2}; \qquad b_2 = \frac{\pi}{L}$$

$$a_1 = \frac{1}{2}(p_0 + p_a); \qquad b_1 = \frac{1}{2}(p_0 - p_a)$$

we got

$$p = \frac{1}{2}(p_0 + p_a) + \frac{1}{2}(p_0 - p_a)\sin(\frac{\pi}{2} + \frac{\pi}{L}x) \tag{13}$$

$$\frac{dp}{dx} = \frac{\pi}{2L}(p_0 - p_a)\cos(\frac{\pi}{2} + \frac{\pi}{L}x) \tag{14}$$

$$\frac{Dp}{Dt} = \frac{\partial p}{\partial t} + \frac{\pi}{2L}u_x(p_0 - p_a)\cos(\frac{\pi}{2} + \frac{\pi}{L}x) \tag{15}$$

2.3 Transfer Flux in ICFB

From the characteristic line equation (12) of quasi-linear first order partial differential (11) and (14),

$$\beta T u_x \frac{\pi}{2L}(p_0 - p_a)\cos(\frac{\pi}{L}x) = \mu\psi + \sum j_i \cdot \phi_i + \sum \frac{\overline{H_i}}{M_i}(\nabla \cdot j_i - r_i) \tag{16}$$

$$\sum \beta_i T u_x \frac{\pi}{2L}(p_0 - p_a)\cos(\frac{\pi}{L}x) = \sum L_i + \sum j_i \cdot \phi_i + \sum \frac{\overline{H_i}}{M_i}(\nabla \cdot j_i - r_i) \tag{17}$$

$$\beta = \sum \beta_i$$

$$\mu\psi = \sum L_i$$

2.4 Flow Model of ICFB and its Numerical Solution

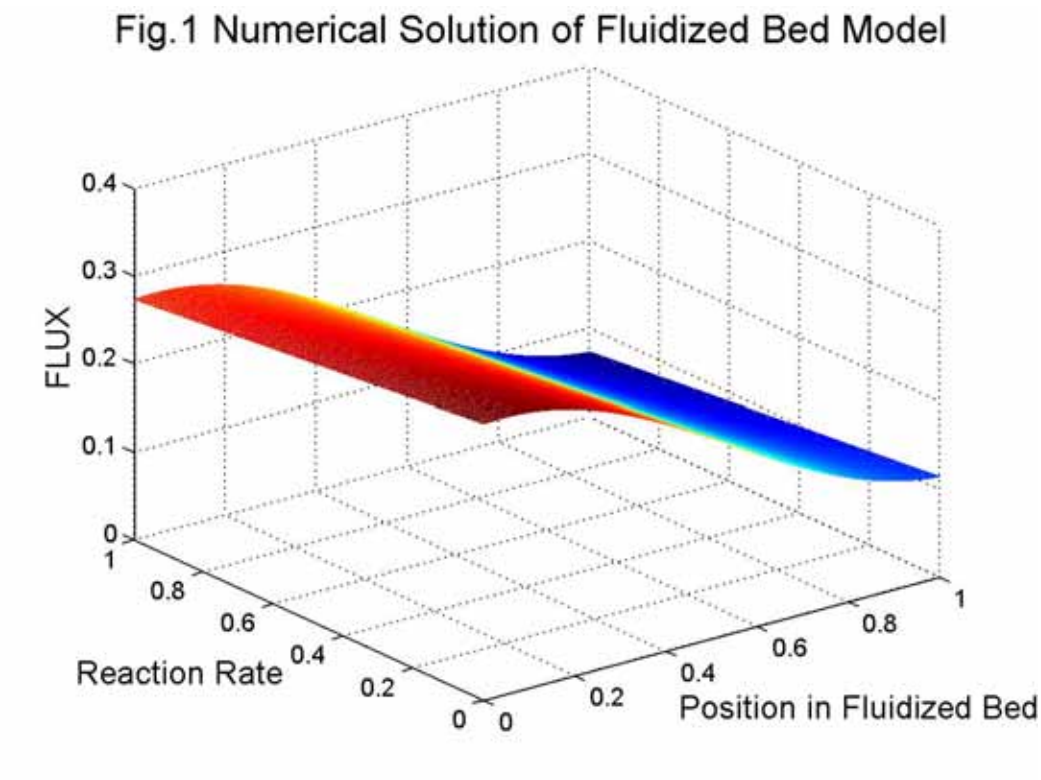
The transfer equation in ICFB has been represented as (17), component i in one

$$j_i = \exp(-\frac{gM}{H}z)\times$$
$$\times\left[\frac{-rH(gML)^2 + ag^2M^3L^2L_i - ag^2M^3L^2 - rH^3\pi^2 + aML_i\pi^2H^2 + J_0g^3M^3L^2 + gJ_0M\pi^2H^2}{\left(g^2M^2L^2 + \pi^2H^2\right)gM}\right] -$$
$$-\frac{ag^2M^3L^2\cos\left(\frac{z}{L}\pi\right) - ag\pi HLM^2\sin\left(\frac{z}{L}\pi\right) + ag^2M^3L^2L_i - aM\pi^2L_iH^2 - g^2M^2L^2rH - r\pi^2H^3}{gM} \tag{18}$$

here, $a = \frac{\beta_i\pi}{2}Tu_x\left(p_0 - p_a\right)$

dimensional could be solved

Fig.1 Numerical Solution of Fluidized Bed Model



2.5 Concentration distribution in ICFB

The mass flux of multicomponents system consist of the parts: concentration diffusion flux

j_i^m, thermal diffusion flux j_i^T; pressure diffusion flux j_i^P and forced flux j_i^Φ, so total flux of *i* can be described as

$$
\begin{aligned}
j_i &= j_i^m + j_i^T + j_i^P + j_i^\Phi \qquad (19)\\
j_i^m &= \frac{c^2}{\rho RT}\sum_{j=1}^{n} M_i M_j D_{ij}^0 \sum_{k=1;k\neq j}^{n} x_j \left(\frac{\partial \mu_i}{\partial x_k}\right)_{T,P} \nabla x_k\\
j_i^T &= 0\\
j_i^P &= \frac{c^2}{\rho RT}\sum_{j=1}^{n} M_i M_j^2 D_{ij}^0 x_j \left(\frac{\overline{V_j}}{M_j}\cdot\frac{1}{\rho}\right)\nabla p\\
j_i^\phi &= \frac{c^2}{\rho RT}\sum_{j=1}^{n} M_i M_j^2 D_{ij}^0 x_j \left(\phi_j - \sum_{k=1}^{n}\frac{\rho_k}{\rho}\phi_k\right)\\
D_{ij} &= D_{ij}^0 \frac{d\ln \alpha_i}{d\ln x_j}
\end{aligned}
$$

while gas-liquid two phase flow was discussed

$$j_A^m = \frac{c^2}{\rho} M_A M_B D_{AB}^0 \left(\frac{\partial \ln \alpha_A}{\partial \ln m_A}\right)_{T,p} \nabla m_A \qquad (20)$$

$$j_A^p = \frac{c^2}{\rho RT} M_B^2 M_A D_{AB}^0 m_A \left(\frac{\overline{V}}{M_j}\frac{1}{\rho}\right)\nabla p \qquad (21)$$

$$j_A^\phi = \frac{c^2}{\rho RT} M_B^2 M_A D_{AB}^0 m_A (\phi_A - \phi_B) \qquad (22)$$

$$
\begin{aligned}
&C_1\nabla m + C_2\cdot\frac{\pi}{2L}(p_0 - p_a)\cos\left(\frac{\pi}{2}+\frac{\pi}{L}x\right)\cdot m = \exp(-\frac{gM}{H}x)\times\\
&\times\left[\frac{-rH(gML)^2 + ag^2M^3L^2L_i - ag^2M^3L^2 - rH^3\pi^2 + aML_i\pi^2H^2 + J_0g^3M^3L^2 + gJ_0M\pi^2H^2}{\left(g^2M^2L^2+\pi^2H^2\right)gM}\right] -\\
&-\frac{ag^2M^3L^2\cos\left(\frac{z}{L}\pi\right) - ag\pi HLM^2\sin\left(\frac{z}{L}\pi\right) + ag^2M^3L^2L_i - aM\pi^2L_iH^2 - g^2M^2L^2rH - r\pi^2H^3}{gM}
\end{aligned}
\qquad (23)
$$

here

$$C_1 = \left(\frac{C^2}{\rho}\right)M_i M_j D_{ij}^0\left(\frac{\partial \ln \alpha_i}{\partial \ln m_i}\right)_{T,P}$$

$$C_2 = \left(\frac{C^2}{\rho RT}\right)M_i^2 M_j D_{ij}^0\left(\frac{\overline{V}}{M_i\rho}\right)$$

2.6 Non Chemical Reaction in ICFB

The characteristic line equation(12) could be expressed as follow if non chemical reaction taken place in ICFB system.

$$\beta T \frac{dp}{dt} = \mu\psi + \sum_{i=1}^{n} j_i \cdot \phi_i + \sum_{i=1}^{n} \frac{\overline{H_i}}{M_i}(\nabla \cdot j_i)$$

$$\beta_i T \frac{dp}{dt} = L_i + g \cdot j_i + \frac{\overline{H_i}}{M_i}(\nabla \cdot j_i) \qquad (24)$$

then

$$j_i = \frac{a_1}{gM} + \exp(-\frac{gM_i}{H_i}x)(\frac{-a_1 H + J_0 gM}{gM})$$

$$a_1 = \frac{\beta TM}{H}\frac{dp}{dt} - \frac{L_i M}{H}$$

r = 0 , take the formula (19)-(22) into (23), and combine with (24), we can obtain the distribution in one dimensional coordinate..

$$m = \exp\left(-\pi a_2 L \cos\left(\frac{x}{\pi L}\right)\right)\int_0^x \frac{\exp\left(-\frac{gM}{H}x\right)a_3 + \exp\left(-\frac{gM}{H}x\right)gJ_0 + a_4}{g}\exp\left(a_2 \pi L \cos\left(\frac{x}{\pi L}\right)\right)dx +$$

$$+\left[\frac{\exp\left(-\pi a_2 L \cos\left(\frac{x}{\pi L}\right)\right)J_0}{\cosh(\pi a_2 L) - \sinh(\pi a_2 L)}\right] \qquad (25)$$

and

$$a_3 = \frac{\pi}{2L}\frac{C_2}{C_1}(p_0 - p_a)$$

$$a_4 = -\frac{a_1 H}{M}$$

Conclusion:

1. A new computational fluid dynamics modeling of inter- circulating fluidized bed has been proposed.
2. Numerical solution of the model is obtained
3. The simulated results are consistent with experiment

List of symbols

1. ρ mass concentration
2. w_i mass fraction of I
3. r_i reaction rate
4. $\overline{H}_i$ partial molar enthalpy
5. $\overline{U}_i$ partial internal energy
6. τ the energy dissipative factor
7. $\mu \ \psi$ means the dissipative energy from internal viscosity
8. D_{ij} diffusion coefficient
9. α_i activity
10. γ coefficient of activity
11. j_i permeate flux
12. L height of ICFB
13. β expanding coefficient

Reference

1. R.W. Fox and A.T. McDonald, *Introduction to Fluid Mechanics,* John Wiley & Sons, 1994.
2. N. Ngampradit, P. Piumsomboon, Simulation of a Circulating Fluidized Bed Combustor with Shrinking Core and Emission Models, *ScienceAsia* 30 (2004): 365-374
3. RW Missen, CA Mims, and BA Saville , Multiphase reacting systems. In: *Introduction to Chemical Reaction Engineering and Kinetics*, pp 224-39 John Wiley & Sons, New York, USA(1999).
4. Gilbertson, M.A. and Yates, J.G., “The Motion of Particles Near a Bubble in a Gas-Fluidized Bed”, *J. Fluid. Mech.*, 323, 377-385 (1996).
5. R Sotudeh-Gharebaagh, R Legros, J Chaouki, and J Paris. Simulation of Circulating Fluidized Bed Reactors using ASPEN PLUS. *Fuel,* 1998, 77, 327-37.
6. L Huilin, B Rushan, L Wenti, L Binxi and Y Lidan , Computations of a circulating fluidized-bed boiler with wide particle size distributions. *Ind. Eng. Chem. Res* 2000 39, 3212-20.
7. V. N. Babak, T. B. Babak, and L. P. Kholpanov, Unsteady-State Mass Transfer of Gases between Two Quiescent Phases, *Theoretical Foundations of Chemical Engineering,* 2004, 38, 462–477.