Computer Simulation of Flow Processes in Fluidized Bed Reactors†

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Abstract

The paper outlines and exemplifies a multi-dimensional multi-phase Computational Fluid Dynamics (CFD) model for the various processes that occur in fluidized bed reactors. The model is based on the Eulerian description of the two phases: gas and particles. This means that separate conservation equations are set up for these phases. Calculations are shown for some examples that include flow patterns in circulating beds.

1. Introduction

1.1 The problem

Many different processes influence the total performance characteristics of fluidized bed reactors. Among these are the gas/particle flow and distribution, chemical reactions, and heat transfer. All these processes occur simultaneously and are intimately coupled to each other. The performance of the reactor is strongly dependent on the interactions between these processes and the geometrical design of the reactor. Because of the complexities of such problems, there are no analytical methods available that can describe in detail what is occurring inside a fluidized bed reactor. In each new reactor it is very often the geometrical details that will determine the performance of the final design of the reactor. Until recently the design of fluidized bed reactors has therefore been based on experimental work done on a laboratory and pilot-plant scale, and on extrapolation of these data to full scale by the application of various empirical scaling techniques.

These design techniques may be very expensive, and give insufficient and inaccurate information about the performance. New computer techniques for fluid flow processes have now made it possible to develop new design methods based on mathematical modelling of the basic processes that occur in the actual geometrical model of the reactor. To apply these methods, the basic conservation equations of flow, chemical reactions, and heat transfer as well as the coupling between them and the coupling between the two phases, must be solved for a multi-dimensional calculation domain.

1.2 Previous work

Gidaspow, has reviewed the CFD models that had evolved up until about 1985. The models at that time had demonstrated the capability to simulate some of the crucial characteristics such as bubble formation and development in bubbling fluidized beds. The models assumed a two-phase gas-particle flow with given apparent viscosities in the gas and in the particle phases. Shih et al., introduced a model that takes account of the multi-sized particle problem and showed application to a sedimentation problem. The work of Tsuo and Gidaspow, showed that the model was able to calculate the flow patterns in circulating fluidized beds. This model had to assume an apparent viscosity for the particle phase to be able to predict the experimentally observed phenomena. The works of Ding and Gidaspow, and Ma and Ahmadi, propose to couple the apparent viscosities in the two phases by introducing turbulence models for each of the phases. A comprehensive model for two-phase flow, heat transfer and chemical reactions in a fluidized bed gasifier has been presented by Gidaspow et al.

1.3 Objectives of paper

The present paper will present a two-phase
multi-dimensional model for the processes that occur in fluidized beds for catalytic chemical reactions. The model will be verified against experimental data for isothermal flow fields in various systems.

2. Governing Equations

2.1 Fluid dynamics model

The governing equations are deduced based on the Eulerian concept. This means that the phases share the space and interact with each other. All equations are such that all volume fractions may take values between zero and one.

Based on the works of Ding and Gidaspow, and Ma and Ahmadi, the following flow model for gas particle flow may be formulated using the following dependent variables: \( \alpha_g, \alpha_p, U_{ig}, U_{ip}, k_i, k_p, \epsilon_i, \epsilon_p \) and \( \rho \). Here the variables have the index \( g \) for the gas phase and index \( p \) for the particle phase. The variables are volume fractions, velocity components, turbulent kinetic energy, dissipation of turbulent kinetic energy and the pressure. Conservation equations written in Cartesian tensor notation may be formulated as:

**Mass balances:**

Gas:

\[
\frac{\partial}{\partial t} (\rho \alpha_g) + \frac{\partial}{\partial x_i} (\rho \alpha_g U_{ig}) = 0
\]  

Particles:

\[
\frac{\partial}{\partial t} (\rho \alpha_p) + \frac{\partial}{\partial x_i} (\rho \alpha_p U_{ip}) = 0
\]  

These equations are valid for catalytic reactions with no mass transfer between the phases.

**Momentum balances:**

Gas:

\[
\frac{\partial}{\partial t} (\rho \alpha_g U_{ig}) + \frac{\partial}{\partial x_i} (\rho \alpha_g U_{ig} U_{ig}) = -\alpha_g \frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_i} (\tau_{ig} + C_{ig}(U_{ig} - U_{ip})) + \alpha_g \alpha_p g_i
\]  

Particles:

\[
\frac{\partial}{\partial t} (\rho \alpha_p U_{ip}) + \frac{\partial}{\partial x_i} (\rho \alpha_p U_{ip} U_{ip}) = -\alpha_p \frac{\partial \rho}{\partial x_i} + \frac{\partial}{\partial x_i} (\tau_{ip} + C_{ip}(U_{ip} - U_{ig})) + \alpha_p \alpha_g g_i + G(\alpha_p) \frac{\partial \alpha_g}{\partial x_i}
\]  

Friction between the phases:

\[
C_{ig} = 15\frac{\alpha_g^2 \delta U_{ig}}{\alpha_g (\delta \rho \Phi_g)^2} + 1.75 \alpha_p \frac{\partial \rho}{\partial x_i} \frac{|V_g - V_p|}{\rho_g \Phi_g}
\]  

when \( \alpha_g < 0.8 \)

\[
C_{ip} = 3 \frac{\alpha_p^2 \delta U_{ip}}{\delta \rho \Phi_g} \frac{|V_g - V_p|}{\rho_p \Phi_g}
\]  

when \( \alpha_g \geq 0.8 \)  

Where \( \Phi_g \) is the form factor of the particles.

\[
C_d = \frac{24}{Re_p} \left[ 1 + 0.15 \cdot Re_p^{0.687} \right] \quad \text{for } Re_p < 1000
\]

\[
C_d = 0.44 \quad \text{for } Re_p > 1000
\]

\[
Re_p = \frac{a_p \rho_p |V_g - V_p|}{\mu_{lam,p}}
\]

Shear stresses are related to the gradients of velocity components and a turbulent viscosity as:

Gas:

\[
\tau_{ig} = \mu_{t,g} \left( \frac{\partial U_{ig}}{\partial x_i} + \frac{\partial U_{ig}}{\partial x_j} \right) - \frac{2}{3} \frac{\partial}{\partial x_i} \frac{\partial U_{ig}}{\partial x_k}
\]

where \( \mu_{t,g} = \mu_{lam,g} + C_{t,g} \alpha_p \rho_p \frac{k_{ij}^2}{\epsilon_g} ; C_{t,g} = 0.06 \)

Particles:

\[
\tau_{ip} = \mu_{t,p} \left( \frac{\partial U_{ip}}{\partial x_i} + \frac{\partial U_{ip}}{\partial x_j} \right) - \frac{2}{3} \frac{\partial}{\partial x_i} \frac{\partial U_{ip}}{\partial x_k}
\]

where \( \mu_{t,p} = C_{t,p} \alpha_p \rho_p \frac{k_{ij}^2}{\epsilon_p} \)

\[
C_{t,p} = 0.0853 \left( (g_p \alpha_p)^{-1} + 3.2 + 12.182 \alpha_p g_0 \right) \quad \text{with}
\]

\[
g_0 = \frac{1}{\left( \alpha_p \right)^{0.678021}} \left[ 1 - \left( \frac{\alpha_p}{\alpha_{p,m}} \right)^{0.65508} \right] \quad (9)
\]

Where \( \alpha_{p,m} \) is the maximum solid volume fraction for a randomly packed bed. \( \alpha_{p,m} \) is taken to be 0.65.

Solid stress is given by:

\[
G(\alpha_g) = \frac{\partial \tau}{\partial \alpha_g}
\]

\[
G(\alpha_g) = G_0 e^{-20(\alpha_g - 0.62)} \quad \text{where } G(\alpha_0) = G_0 = 1.0 \quad \text{when } \alpha_g = 0.62
\]

Turbulent kinetic energy:

Gas:

\[ G(\alpha_g) = \frac{\partial \tau}{\partial \alpha_g}
\]

\[ G(\alpha_g) = G_0 e^{20(\alpha_g - 0.62)} \quad \text{where } G(\alpha_0) = G_0 = 1.0 \quad \text{when } \alpha_g = 0.62
\]
Here, the effective transport coefficients are related to the turbulent viscosities as:

\[
\Gamma_{k,\nu} = \mu_{t,\nu} \quad \text{and} \quad \Gamma_{\tau,\rho} = \mu_{t,\rho}
\]

(13)

Dissipation of turbulent kinetic energy:

Gas:

\[
\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho U_i \varepsilon) =
\frac{\partial}{\partial x_i}\left[\Gamma_{\varepsilon,\rho} \frac{\partial \varepsilon}{\partial x_i}\right] + C_{\varepsilon,\rho} \left(\frac{\varepsilon}{k}\right) \left[\tau_{\varepsilon,\rho} \frac{\partial U_i}{\partial x_i} + 2 \cdot C_{\rho,\tau} \left(k_\rho - c \cdot k_\rho\right)\right] - \langle \rho \partial \rangle \sigma_\varepsilon
\]

(14)

Particles:

The dissipation in the particle phase is given by an algebraic equation as:

\[
\varepsilon_p = 3.9 \rho_0 \dot{q}_0 \left(1 - r^2\right)^{3/4} k_\rho
\]

(15)

where \(r\) is the restitution.

Here, the effective transport coefficient is related to the turbulent viscosity as:

\[
\Gamma_{k,\varepsilon} = \frac{\mu_{t,\varepsilon}}{1.3}
\]

(16)

and

\[
c = \frac{1}{1 + \left(\frac{1}{C_{\rho,\tau} T_i}\right) \frac{k_\rho}{\varepsilon_\rho}}
\]

(17)

2.2 Heat transfer model

The heat transfer is taken account of by solving the two energy equations for the two phases where heat is generated by the exothermic (homogeneous) gas phase chemical reactions and then transported between the phases.

These equations are:

Gas:

\[
\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho U_i h) =
\frac{\partial}{\partial x_i}\left[\Gamma_{h,\rho} \frac{\partial h}{\partial x_i}\right] + h_{\nu,\rho}(T_p - T_\rho) + \sum \Delta H_k \gamma_k
\]

(18)

Particles:

\[
\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_i}(\rho U_i h) = \frac{\partial}{\partial x_i}\left[\Gamma_{h,\rho} \frac{\partial h}{\partial x_i}\right] + h_{\nu,\rho}(T_p - T_\rho)
\]

(19)

Here, the effective transport coefficients are related to the turbulent viscosities as:

\[
\Gamma_{h,\nu} = \frac{k_{\nu,\rho}}{C_{\nu,\rho} \mu_{t,\rho}} \quad \text{and} \quad \Gamma_{h,\tau} = \frac{\mu_{t,\tau}}{0.7}
\]

(20)

where \(k_{\nu,\rho}\) is the laminar conductivity of the gas and \(c_{p,\rho}\) is the specific heat of the gas.

The volumetric heat transfer coefficient \(h_{\nu,\rho}\) is calculated as:

The basis for calculating the volumetric heat transfer coefficient is based on correlations of the Nusselt number \(N_p\) in the various flow regimes characterized by the Reynolds number and volume fraction of gas according to:

If \(a_\rho \leq 0.8\)

\[N_p = 2 + 0.106 \cdot Re \cdot S_p \quad Re \leq 200\]

\[N_p = 0.123 \left(\frac{4 \cdot Re}{Sp^{0.17}}\right) \cdot Sp^{0.83} \quad 2000 \geq Re > 200\]

\[N_p = 0.61 \cdot Re^{0.67} \cdot Sp \quad Re > 2000\]

If \(a_\rho > 0.8\)

\[N_p = (2 + 0.16 \cdot Re^{0.67}) \cdot Sp \quad Re \leq 200\]

\[N_p = 8.2 \cdot Re^{0.58} \cdot Sp \quad 1000 \geq Re > 200\]

\[N_p = 1.06 \cdot Re^{0.457} \cdot Sp \quad Re > 1000\]

where

\[Re = \frac{\rho_0 \cdot d_p \cdot \left(V^2 - V_0^2\right)}{\mu_m \cdot \rho_0}
\]

\[S_p = \frac{\rho_0 \cdot d_p}{\kappa_{\nu,\rho}}
\]

\[N_p = \frac{h_{\nu,\rho} \cdot d_p}{\kappa_{\nu,\rho}}
\]
2.3 Chemical reaction model

Since chemical reactions are only taking place in the gas phase, only species conservation for this phase is needed. These are:

\[
\frac{\partial}{\partial t} (\rho a Y_j) + \frac{\partial}{\partial x_i} (\rho a U_i Y_j) = \frac{\partial}{\partial x_i} \left[ \Gamma_{Y_j,a} \frac{\partial Y_j}{\partial x_i} \right] \\
= \frac{\partial}{\partial x_i} \left[ r_{i,g} \frac{\partial Y_j}{\partial x_i} \right] + a \rho r_{i,c} + a \rho r_{i,c} \tag{22}
\]

Here, \( r_i \) is the net bulk gas-phase reaction rate for component \( j \), and \( r_{i,c} \) is the gas phase reaction occurring on the surface of the catalyst particle for component \( j \). The effective gas-phase transport coefficient is calculated as:

\[
\frac{\partial}{\partial x_i} \left[ \Gamma_{Y_j,a} \frac{\partial Y_j}{\partial x_i} \right] + a \rho r_{i,c} + a \rho r_{i,c} \tag{23}
\]

\( \Gamma_{Y_j,a} \) is the molecular diffusivity of the gas-phase component with mass fraction \( Y_j,a \).

3. Solution Procedure

Solution of the set of partial differential equations given above is performed by finite-domain methods. The calculation method is taken from the work of Spalding. The calculation domain is divided into a finite number of main grid points where pressure, densities, void fractions, turbulent quantities, enthalpies and mass fractions of the chemical species are stored. The velocity components are, on the other hand, stored at grid points located midway between the main grid nodes. The relevant conservation equations are integrated over control volumes surrounding the relevant grid points in space and over a time interval. This integration is performed using upward differencing in space and implicit differencing in time. The result of this is a set of non-linear algebraic equations which are solved by the application of the well known Tri-Diagonal Matrix Algorithm (TDMA) used along the various coordinate directions. For the void fraction and velocity equations, a point iteration method is used. Special care has been taken to solve the coupling of the momentum equations with the continuity equations. For this we use the so-called IPSA procedure proposed by Spalding. The Partial Elimination Algorithm (PEA) is used to de-couple the drag force between the phases in the momentum equations.

4. Simulations

Parts of the model given above are compared against two isothermal non-reacting gas-particle flow situations. In the present paper, focus has been directed towards calculating the flow fields and particle distributions and comparing the predictions with data from literature and data generated in our own laboratory using Laser-Doppler Anemometry (LDA). The first case is related to a core annulus type flow in an 11-m-high, 0.305-m diameter tube of Bader et al., and the second is related to our own laboratory setup of a 1-m-high, 0.03-m diameter circulating fluidized bed.

CASE 1: Large-scale tube of Bader et al.

The particles used in this study had a diameter of 76 \( \mu \)m, a density of 1714 kg/m\(^3\) and a sphericity of 1.0. The tube was initially empty and the flow was started at the inlet with flow velocities of 0.228 m/s for the particles and 3.7 m/s for the gas. The particle volume fraction at the inlet was fixed at 0.25. The calculation was performed using a Cartesian description with 76 grid points along the height and 30 grid points across the diameter. It took about 14 seconds to fill the empty tube. Fig. 1 gives an overview of the results of stream lines for gas, particles and distribution of volume fraction of particles at 16 seconds after start-up. Please note that the contours are expanded in the transverse direction to improve visualisation of the details. It was generally found that the flow did not reach a true steady state situation, but had a cyclic behaviour. The general trend was that the gas and particle flow had an upward flow in the centre of the tube and a downward flow along the wall. Bader et al., had measured profiles across the tube diameter of both volume fraction of gas (porosity) and particle velocity. Fig. 2 and Fig. 3 show comparisons between measured and predicted profiles at a height of 9.1 m from the inlet. The predicted profiles were determined by averaging over 5 seconds. Fig. 2 shows that the porosity is well predicted, whereas the particle velocity profile in Fig. 3 shows some discrepancies between
Fig. 1 Contours of stream lines of gas and particles and volume fraction of particles.

Fig. 2 Measured and predicted profiles of gas volume fraction (porosity) as a function of distance across the tube diameter at 9.1 m from the inlet.

Fig. 3 Measured and predicted profiles of particle velocity as a function of distance across the tube diameter at 9.1 m from the inlet.
experiments and predictions. The general trend seems, however to be well predicted, namely upward flow in the centre and downward flow along the wall.

**CASE 2: Laboratory-scale circulating fluidized bed**

The vertical particle flow velocity in the lab-scale fluidized bed reactor was determined by a laser Doppler anemometer delivered by Dantec. This system made it possible to measure both positive and negative particle velocities. Velocity profiles across the tube diameter were measured at three different heights above the distributor plate. The average particle diameter was about 55 \( \mu \text{m} \) and the density was 1600 kg/m\(^3\). The particles that were transported from the reactor were separated in a cyclone and directed back into the fluidized bed just above the distributor plate. The gas superficial velocity was 1.7 m/s.

The calculation was performed using a Cartesian description. The calculation domain included both the vertical tube and the separator and return tube. 102 grid points were used in the axial direction and 26 points were used in the radial direction.

**Fig. 4** shows the predicted contours of volume fraction of particles, particle and gas streamlines. The figure shows that the gas and particles are flowing upwards in the centre of the tube and have regions with negative velocities. The figure also shows a significant slip between the gas and particle flow. This is especially seen in the separation section of the flow system. **Fig. 5** shows a comparison between the measured and predicted profiles of the vertical particle velocity at three different heights above the distributor plate. It is seen that the overall agreement is good, i.e. the flow is upward in the centre of the tube and is directed downwards along the wall. However, the negative velocity is overpredicted.

**Discussion**

The comparisons between measurements and predictions in the two cases given above are reasonable. However, more work is needed to improve the model. This is particularly so for the turbulence model that determines the effective viscosity for the two phases. It must also be mentioned that the simulations were performed with a Cartesian geometry description, whereas the geometry is axisymmetric. Calculations
should therefore also be performed using an axisymmetric geometry description.

5. Concluding Remarks

A comprehensive multi-dimensional CFD model for gas/particle flow, heat transfer and chemical reactions in fluidized bed reactors has been proposed. The model is incorporated in a 2D computer code and some initial verification simulations of isothermal flows have been carried out. The predictions give reasonable agreement with data from literature and our own experimental data. However, more model development is still needed especially with regard to turbulence modeling. In addition to this, the model needs to be tested against experimental data where chemical reaction and heat transfer is included.

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7. Nomenclature

c : constant
c_{p,g} : specific heat for gas
C_{pg} : gas - particle friction coefficient
C_{d} : drag coefficient
C_{v}, \zeta, \zeta_{v} : constants in turbulence model
d_{p} : particle diameter
D : molecular gas diffusivity
g_{i} : j-direction component of gravity acceleration
g_{0} : radial distribution modulus
G : solid stress modulus
h_{g,p} : gas and particle enthalpy
h_{v,g} : volumetric heat transfer coefficient
\Delta H_{k} : heat of reaction for reaction no. k
k_{g,p} : kinetic energy of turbulence in gas and particle phase
N_{p} : Nusselt number
p : pressure
r_{g}, r_{p} : gas phase reaction rate in the bulk phase and on the surface of the particles
r : restitution factor
Re_{p} : Reynolds number
S_{p} : specific surface area of particles
t : time
T_{g}, T_{p} : gas and particle temperature
T_{L} : Lagrangian time scale of turbulence
U_{g,p} : j-component of velocity for gas and particles
\nabla_{g}, \nabla_{p} : velocity vector for gas and particles
X_{i} : coordinate direction in i-direction
Y_{j,i,d} : mass fraction of component j in the gas phase

Greek

\alpha_{g}, \alpha_{p} : gas and particle volume fraction
\Gamma_{g}, \Gamma_{+2} : effective turbulent transport coefficient for scalar variable \Phi
\delta_{g} : Kroenecker delta
delta_{g}, \delta_{p} : dissipation of kinetic energy of turbulence
\kappa : molecular thermal conductivity
mu_{g}, \mu_{p} : turbulent viscosity of gas and particles
rho_{g}, \rho_{p} : density of gas and particles
\tau_{ij,g}, \tau_{ij,p} : stress tensor in gas and particle phases
\Phi_{g} : form factor of particles
Subscripts

\( g \) : gas phase
\( \text{lam} \) : laminar
\( p \) : particle phase
\( t \) : turbulent

References

1) Gidaspow, D.: Hydrodynamics of fluidization and heat transfer, Super-computer modelling, Appl. Mech. Rev., Vol 39, 1(1986), 1-23
2) Shih, Y.T., Gidaspow, D., and Wasan, D.T.: Hydrodynamics of sedimentation of multi-sized particles, Powder Technology, Vol. 50, (1987), 201-215
3) Tsuo, Y.P and Gidaspow, D.: Computations of flow-patterns in circulating fluidized beds, AIChE Journal, Vol. 36, (1990), 885-896
4) Ding, J. and Gidaspow, D.: A bubbling fluidization model using kinetic theory of granular flow, AIChE Journal, Vol. 36, (1990), 523-538
5) Ma, D. and Ahmadi, G.: A thermodynamical formulation for dispersed multi-phase turbulent flows - Part II: Simple shear flows for dense mixtures, Int. J. Multi-phase Flows, Vol. 16, (1990), 342-351
6) Gidaspow, D., Ettehadieh, B., and Bouillard, J.: Hydrodynamics of fluidization: Bubbles and gas compositions in the U-gas process, AIChE Symposium Series No. 241, Vol. 80, (1985), 57-64
7) Spalding, D.B.: Computer simulation of two-phase flows with special reference to nuclear reactor systems, Computational techniques in heat transfer, Ed.: R.W. Lewis, K. Morgan, J.A. Johnson and W.R. Smith, Pineridge Press, 1985, 1-44
8) Bader, R., Findlay, J., and Knowlton, T.M.: Gas/solid flow patterns in a 30.5-cm-diameter circulating fluidized bed, 2nd Int. circulating fluidized bed conference, March 14-18, Compiègne, France, 1988.