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# NUMERICAL MODELING OF GAS-SOLIDS FLOW IN LARGE SCALE CIRCULATING FLUIDIZED BED USING SUBGRID-SCALE MODEL

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## ABSTRACT

Multiphase flows in circulating fluidized bed (CFB) furnaces are heterogeneous and complex in nature. 3D simulations of gas-solids flow in fluidized beds are usually performed using Eulerian description of phases. In this type of modeling approach, the calculation meshes should be fine enough to resolve the small scale flow structures of the flow field. For the sake of affordable computational time, such kind of simulations is always performed using coarse meshes. Inaccurate coarse mesh simulations result into too uniform solids concentration fields, and as a consequence, the gas-solid drag force is overestimated which leads to higher solids circulation rate. Thus, there is a need to formulate suitable correction for gas-solid drag force. In this work, a space averaging approach was used to formulate the subgrid-scale model for gas-solid drag force which was used for coarse mesh simulations of a large scale CFB furnace.

## INTRODUCTION

Large scale circulating fluidized bed furnace is widely used as a chemical reactor in energy industries. In spite of several advantages with its operation, detailed understanding of complex gas-solids flow is still lacking. Thus, such large scale industrial unit requires proper modeling for its better understanding, design and scale-up.

3D large scale numerical simulations of gas-solids flow in fluidized beds are usually performed using Eulerian description of phases. In this kind of modeling approach, both the phases are treated as interpenetrating continua. Such a modeling approach is called as “two-fluid model” approach, details about which can be found in the literature (1, 2). Continuity and momentum equations are solved for both phases. The solid phase momentum equation is closed by the use of kinetic theory of granular flow (2, 3).

In this type of modeling approach, the calculation meshes should be fine enough to resolve the small scale flow structures of the flow field. Such fine meshes for the simulation of fluidized beds, results into a huge number of computational control volumes. For the sake of affordable computational time for 3D large scale fluidized bed studies, such kind of simulations are always performed using coarse meshes. Coarse mesh simulations are performed over large control volumes which results into loss of information about the small scale flow structures of the flow field.

Several research groups have worked for the formulation of closure models which can be used for coarse mesh simulations, but only very few papers exist in the literature which shows simulation of large scale industrial fluidized beds. For example, Zhang et al. (4) performed the 3D simulation of full loop circulating fluidized bed boiler using the EMMS based model for the correction of the gas-solid drag force. Shah et al. (5) performed the 3D simulation of CFB furnace using two solid phases and was simulated using the maximum mesh size of about 0.3 m.

Inaccurate coarse mesh simulations result into too uniform solids concentration fields. As a consequence, the gas-solid drag force is overestimated (Agrawal et al. (6)), which leads to higher entrainment of solids resulting to too high solids concentration at the upper part of the furnace (Shah et al. (7)). Thus, there is a need to formulate suitable expression for gas-solid drag which can be used in numerical simulations of large scale CFB furnaces with a coarse calculation mesh.

Different approaches have been used by the researchers for the formulation of appropriate subgrid-scale models which can be used in coarse mesh simulations. Space averaging approach is used in this work to formulate the subgrid-scale model for gas-solid drag force which is previously presented in the literature (Shah et al. (7)). In this approach, fine mesh simulation is performed using two-fluid model and the results are space averaged to derive the subgrid-scale models which can be used in coarse mesh simulations.

In this work, a numerical modeling study of a large scale industrial CFB furnace is presented. Both coarse mesh simulations with and without subgrid-scale model for the gas-solid drag force are presented. The simulated solid concentration profiles are compared with the empirical data based on pressure profile measurements.

## **METHODOLOGY**

### **Model Setup**

The object of the study was the same CFB unit, which was modeled earlier by Shah et al. (5). The model domain is presented in Fig. 1. The height of the furnace was 43.3 m and the cross-section 14.3 m x 6.7 m. The cell dimensions were about 0.1...0.3 m and the number of calculation cells was about 400 000, using hexahedral cells for most of the domain and tetrahedral cells for tapered lower furnace section.

The model boundaries included primary air through grate, secondary air through multiple secondary air nozzles and other ports, and solid feed rates from the solid circulation ports. The inlet values were based on measured test balance values and on design data. The model did not include any reactions. The furnace temperature and the expansion of colder inlet gases were simulated by setting the solid phases to a fixed temperature (1150 K), specifying the gas inlet temperatures (490 K) and modeling the heat transfer between the gas and solids.

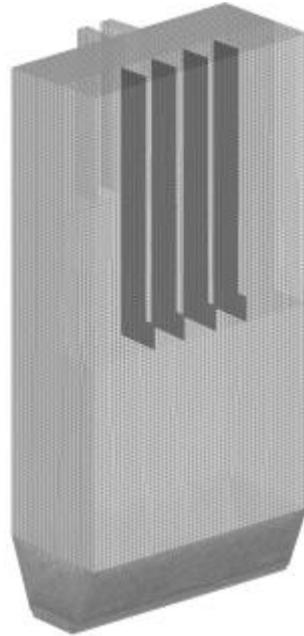


Fig. 1. Model domain.

In the earlier study (Shah et al. (5)), the bed material was simulated as a mixture of two solid phases with fine and coarse particle size (128 and 1500  $\mu\text{m}$ ). The higher solid concentration at the bottom of the furnace was thus achieved with the presence of the coarse solid phase. In this study, the modeling was attempted with a single solid phase with particle diameter 175  $\mu\text{m}$ , which corresponded with the measured average particle size of the bed. Based on pressure profile measurements, the total bed inventory was 50 000 kg, which was controlled in the model by adjusting the feed rate from the return leg chutes.

### Numerical Simulations

Numerical simulations of gas-solids flow were performed in the commercial code, Ansys Fluent 13 applying a two-fluid model based on kinetic theory of granular flow. The simulation parameters and the closure models used in this study are given in Table 1.

Table 1: Material properties and model parameters for the numerical simulations.

Material Properties		Closure models	
Gas phase:	Incompressible ideal gas Molecular weight = 28.872 kg/kmol $\mu = 4.37\text{E-}05$ kg/ms	Interphase momentum exchange coefficient:	Gidaspow
Solid phase:	Diameter = 175E-06 m Density = 2500 kg/m <sup>3</sup>	Heat transfer coefficient:	Gunn
Restitution coefficient: 0.9		Granular viscosity:	Syamlal-Obrien
		Granular bulk viscosity:	Lun-et-al
Mesh and time step sizes		Granular temperature:	Algebraic
Mesh size (m):	0.1 – 0.3	Solids pressure:	Lun-et-al
Time step size (s):	0.001	Radial distribution:	Lun-et-al

The interphase momentum exchange coefficient was modeled by a correlation proposed by Gidaspow et al. (8), which is a combination of Wen and Yu (9) model and Ergun equation (10) model. The simulations were allowed to reach the stable state conditions in which the outlet mass flow rate appears to be stable. After that, the time averaging of the results was performed over 60 s of simulation time. First order implicit for time-stepping and first order upwind for other terms were used as the discretization schemes. The phase coupled SIMPLE algorithm was used for pressure-velocity coupling. The number of iterations per time step was set as 10. With these settings, the residuals behavior was showing acceptable numerical convergence and the relative error between two successive iterations for each scaled residual component was below 1e-03. At the walls, the free slip boundary condition was used for gas phase and the partial slip boundary condition of Johnson and Jackson's model (11) with a value of specular coefficient as 0.001 was used for the solid phase. Two calculation cases were performed: Case 1 with uncorrected drag model and Case 2 with applying a correction of drag term as described in the following chapter.

### Subgrid-scale Model

It is well known that the numerical simulations with the two-fluid model are dependent on the mesh and time step sizes. Thus, there is a need to formulate macroscopic set of equations which can be used for coarse mesh simulations. In this approach, space averaging method was used to derive the subgrid-scale model for the gas-solid drag force. This kind of approach is presented in the literature where simulation results obtained with fine meshes are averaged to derive constitutive correlations which can be used for coarse meshes (7, 12).

In this study, the principle was to determine a term  $\omega$ , which could be used as a correcting factor for the drag coefficient  $K_{gs}$  between the gas and solids:

$$K_{gs} = \omega K_{gs,0} \quad (1)$$

In above, the  $K_{gs,0}$  is the uncorrected drag coefficient produced by the drag model of Gidaspow et al. (8). The data generated by Shah et al. (7) was applied to determine the correction factor  $\omega$  as a function of volume fraction of solids and the distance from wall. In the earlier study (7), the different averaging sizes up to 0.05 m were used and the results clearly showed how the correction factor needs to be smaller as the averaging size increases. In the current study, the maximum cell size was up to 0.3 m. Thus, it is evident that even the values produced with the largest averaging size (0.05 m) might not produce small enough values of  $\omega$  for this case.

Fitting the data for the 0.05 m averaging size, a following correlation was derived:

$$\omega = \omega_{min} + \frac{(1-\omega_{min})}{\varepsilon_{max}} \left[ (\varepsilon_{max} - \varepsilon) \exp\left(-a_1 \frac{\varepsilon}{\varepsilon_{max}}\right) + \varepsilon \exp\left(-a_2 \frac{(\varepsilon_{max}-\varepsilon)}{\varepsilon_{max}}\right) \right] \quad (2)$$

$$\omega_{min} = p [1 - \exp(-q x)]$$

$$a_1 = m \exp(-n x)$$

$$a_2 = 3.5, m = 50, n = 10, p = 0.5, q = 20$$

In above, the  $\varepsilon$  is the volume fraction of solids,  $\varepsilon_{max}$  is the maximum packing density (= 0.63),  $x$  is the distance from wall as absolute value in meters. The rest of the terms are correlation parameters, which have been specified above.

Fig. 2 presents a comparison between the points of  $\omega$  defined from the averaging study (7) and the above correlation. With all data sets, the correction factor approaches unity as the volume fraction of solids approaches zero or packing density, and the value of correction factor is smaller as the distance from wall is smaller. In the achieved data points, there is a clear step change at solid volume fraction 0.2, which corresponds with the step change in the Gidaspow's correlation. The correction factor is probably depending on other variables as well, for example the slip velocity, but for this initial study, this simple correlation was applied.

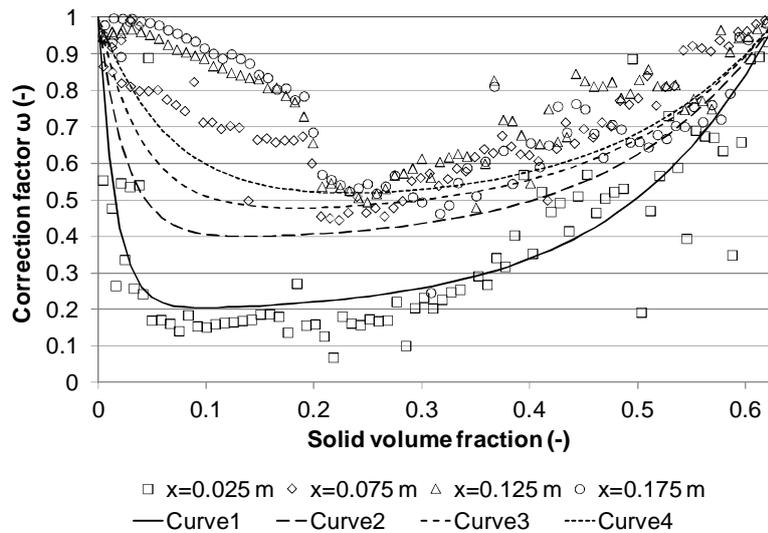


Fig. 2. Correction factor  $\omega$ . The points represent the determined values from small scale studies at different distances  $x$  from wall. The curves represent the derived correction factor curves (Eq. 2) calculated with the same distances ( $x = 0.025, 0.075, 0.125, \text{ and } 0.175 \text{ m}$ ).

## RESULTS AND DISCUSSION

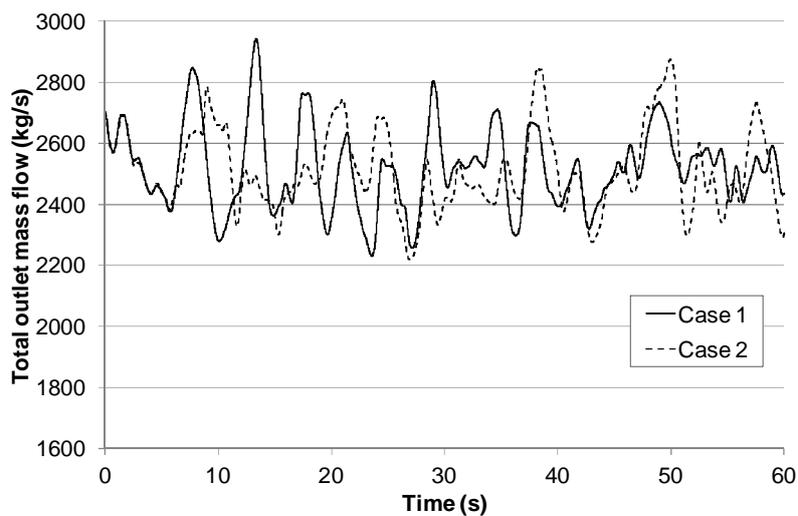


Fig. 3. Total outlet mass flow as function of time.

Fig. 3 presents the total mass flow at the outlets of the furnace for the two cases during the 60 seconds of averaging time. The applied correction factor does not seem to have any significant effect on the outlet mass flow. The reason for the small effect is explained by the following figures. Fig. 4 compares the time averaged volume fraction of solids at a cross-section, which coincides with one return leg chute. Due to relatively small particle size and bed inventory, the flow is quite dilute. In most parts of the furnace, the volume fraction of solids is less than 0.02. With this kind of dilute flow, the values of correction factor are close to unity except for areas close to walls. This is further illustrated in Fig. 5, which shows instantaneous values of solid volume fraction and correction factor.

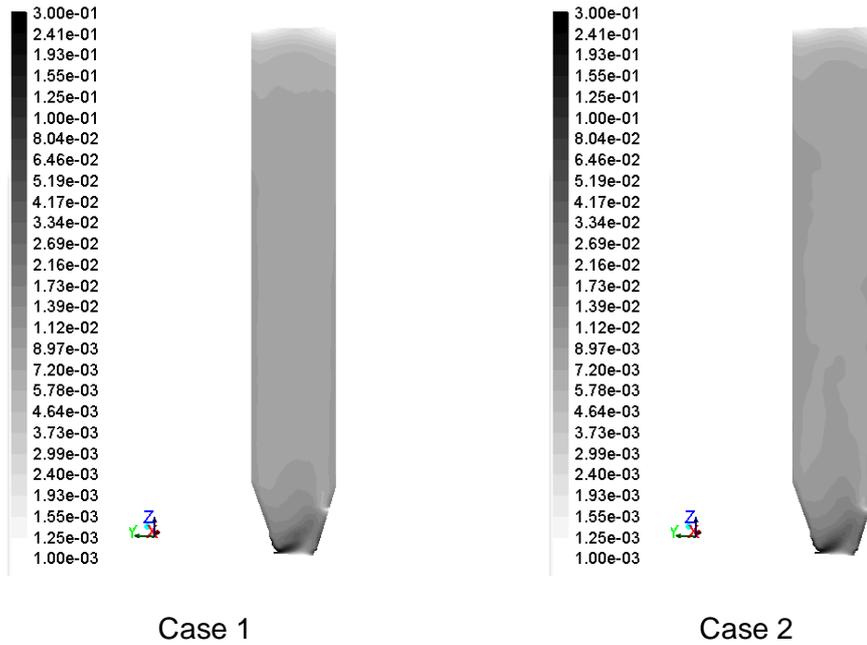


Fig. 4. Time averaged volume fraction of solids at cross-section  $x=3$  m.

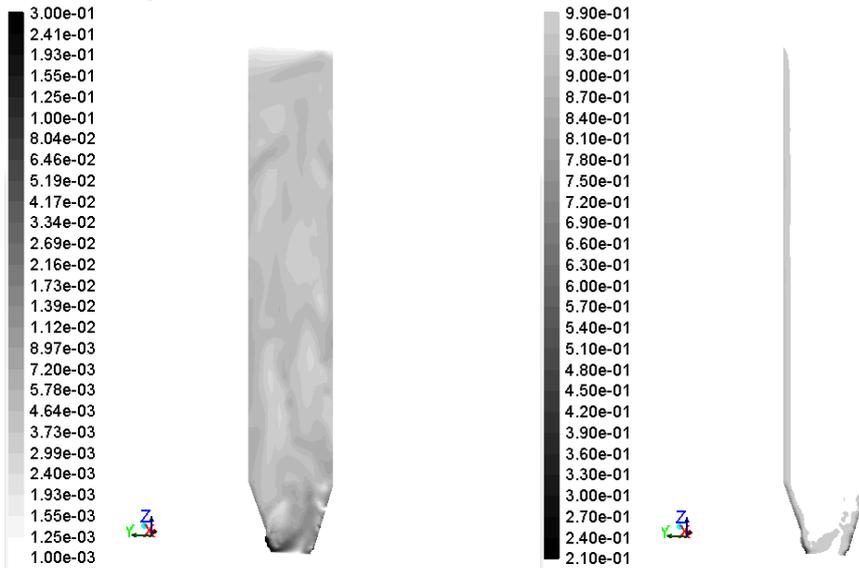


Fig. 5. Instantaneous volume fraction (left) and correction factor  $\omega$  (right) at cross-section  $x=3$  m in Case 2.

As a consequence, the time averaged vertical solid concentration profile in Case 2 is fairly much the same as in Case 1. Fig. 6 compares the vertical volume fraction of solids to values derived from pressure profile measurements. This figure clearly demonstrates the problem: with the existing drag model, the volume fraction of solids is too small at the bottom of the furnace and too high at the top part of the furnace. Unfortunately, the applied correction factor is not enough to change the situation.

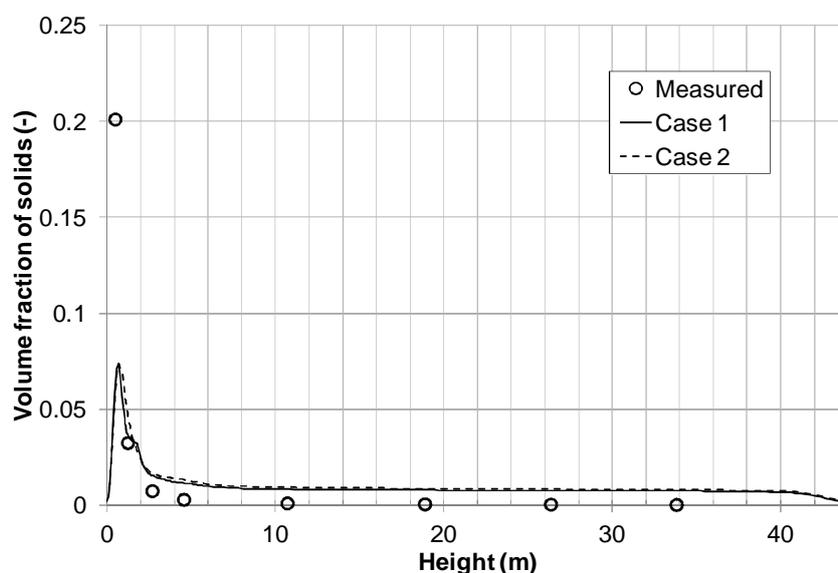


Fig. 6. Time averaged vertical profiles of volume fraction of solids. Comparison of modeled and measured results.

The distance from wall was included as an absolute value. It is possible that in a large scale 3D case, the distance from wall cannot be defined similarly as in small scale 2D case. However, at the moment there is no uniform expression for a dimensionless distance from wall, which could be applied both in cold and hot conditions.

The reason for the small effect in Case 2 is clear: in this case the flow is very dilute. The situation might have changed, if the initial conditions had been different, i.e. with a higher volume fraction of solids at the bottom of the furnace. This could have then produced a different stable state, in which the solids profile had been closer to the measured profile.

Another explaining factor is the cell size: in this calculation, the cell size was clearly higher than in the studies, which were the basis for the correction factor, thus, the values of  $\omega$  should have been smaller. Yet another possible explanation is the applied bed inventory. In this study, the amount of bed inventory was based on measured pressure profile. However, the actual bed inventory can be larger due to fact that part of the solids is not fluidized by hydrodynamic forces but supported by the bottom of the furnace.

## CONCLUSIONS

Based on 2D calculations, a correction of the drag force is needed and the amount of correction depends on the cell size and distance from wall. In the 2D analysis, the maximum cell size was limited to 0.05 m. In the 3D study, the cell size was up to 0.3 m, but the calculations were attempted by using the same correction, which was derived from 2D studies with 0.05 m cell size. In this case, the calculation with one solid phase and a relatively fine particle size produced small volume fraction of solids. Consequently, the effect of the correction factor was limited. Based on the results, the applied correction is not enough to produce results, which would match with the measurements. The different options for correcting the situation will be investigated in the future calculation studies.

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