# Application of CFD to Fluidised Bed Systems

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## ABSTRACT

Fluidised bed systems have the potential to be widely used in the power generation, mineral processing and chemical industries. One factor limiting their increased use is the lack of adequate design techniques for scaling such systems.

A model has been developed for simulating gas-solid fluidised bed plant using the commercial CFD code CFX (formerly CFDS-FLOW3D). The model uses a multiphase Eulerian-Eulerian technique to predict the transient behaviour of fluidised bed plant. To overcome the problem of accurate geometrical representation experienced in previous models a body fitted grid system is employed.

The model is used to predict isothermal flow in a three dimensional bubbling bed and in a two dimensional circulating fluidised bed. Predictions of the three dimensional model show bubble formation with gas bubbles or voids preferentially moving along the centre of the bed. CFB model results show the formation of clusters and a core-annular flow structure in the riser. Solids recirculation is accounted for by modelling the entire CFB loop. Reaction kinetics for coal gasification are included in the model and results are presented for a slugging coal gasifier. Outlet gas predictions are in reasonable agreement with experimental data.

## 1. INTRODUCTION

Bubbling and circulating fluidised bed systems are becoming an increasingly important technology for the power generation, mineral and chemical processing industries. Benefits in economic, operational and environmental terms can be achieved with fluidised bed technology over more traditional technologies. The complex fluid mechanics in fluidised bed systems poses a significant challenge and a technological risk to plant designers and investors.

Current techniques for scaling fluidised beds rely on either scaling laws based on dimensional analysis or simple empirical correlations. In systems with well known behaviour these techniques allow changes in operating parameters to be analysed. However where large changes in scale or operating parameters occur such techniques are often inadequate. For single phase flows CFD modelling has proved capable of overcoming such problems and often provides significant insights into the understanding how the flow behaves.

Early CFD models of fluidised bed systems used specially written codes usually which are limited to two dimensional isothermal flows and simple rectangular geometries. Recent work has extended the Eulerian-Eulerian model in the commercial CFD code CFX (CFDS, 1994) to model fluidised bed systems. An advantage of using CFX is that its multi-block facility and body fitted coordinates allow more complex geometries to be handled than was possible in earlier models. Also, advanced numerical techniques developed for single phase flows can be adopted more readily for use in multiphase flow problems.

This paper demonstrates the application of CFD modelling to a number of typical fluidised bed systems. To demonstrate the model's generality, predictions are presented for a three dimensional bubbling bed, a two dimensional circulating fluidised bed and a slugging fluidised bed coal gasifier.

## 2. NOMENCLUTURE

- $\mathbf{g}$ gravitation vector
- $P$ pressure
- $S$ additional mass source
- $Sc$ additional momentum source
- $\mathbf{u}$ velocity vector
- $\alpha$ volume fraction
- $\beta$ interphase momentum transfer coefficient
- $\rho$ density
- $\mu$ dynamic viscosity

## 3. MODELLING TECHNIQUE

By averaging particle and gas properties over space and time, continuum equations can be derived to approximate the behaviour of both gas and solid particles in a fluidised bed (Gidaspow, 1994). In the present work a single solid and gas phase is assumed, leading to a two phase Eulerian-Eulerian model with particles of a fixed diameter. The commercial finite volume program, CFX (formerly known as CFDS-FLOW3D), is used to solve the continuum equations on a collocated grid. Calculations are performed using SPARC 10 and CRAY Y-MP EL computer platforms located at Swinburne University of Technology and the CRC New Technologies for Power Generation from Low-Rank Coal.

### 3.1 Hydrodynamic Model

Applying principles of mass and momentum conservation to the individual phases allows the following continuum equations for volume fraction and velocities to be derived;

$$\frac{\partial(\alpha_i \rho_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{u}_i) = S_i \qquad (1)$$

$$\begin{aligned}&\frac{\partial(\alpha_i \rho_i \mathbf{u}_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i \ \mathbf{u}_i \ \mathbf{u}_i) \\ &- \nabla \cdot \left\{ \alpha\mu \left[ \nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}} \right] \right\}_i = \\ &- \alpha_i \nabla P + \beta_i (\mathbf{u}_s - \mathbf{u}_g) + \alpha_i \rho_i \mathbf{g} + Sc_i\end{aligned} \qquad (2)$$

where $i = g$ (gas), $s$ (solid). Additional source terms in both equations are required when there is mass transfer between phases as occurs in the gasification model. Constitutive relationships are required for the interphase drag term and are based on the Ergun equation in dense regions and a modified form of single particle drag correlations in leaner regions. To replicate the force acting between particles as particle concentrations approach the particle's packing fraction a solid phase pressure term is added to the solid phase momentum equations. Witt and Perry (1996) provide details of these constitutive relationships.

### 3.2 Gasification Model

The chemistry involved in converting coal into combustible gaseous products is complex, involving a number of different reactions with numerous intermediate stages. A detailed understanding of all reaction and intermediate stages in the gasification process for all coal types and operating conditions is not presently available. Furthermore, inclusion of such detail would require considerable computational resources. To enable results to be obtained based on current knowledge, a simplified reaction scheme is used and a number of simplifying assumptions introduced. The main assumptions are that coal particles are mono-sized, devolatilisation is instant with volatiles entering as gaseous species and the solid material consists only of ash and coal char. Chemical reactions in the model are;

$$C + O_2 \rightarrow CO_2 \qquad \text{(I)}$$

$$C + \tfrac{1}{2} O_2 \rightarrow CO \qquad \text{(II)}$$

$$C + H_2O \rightarrow CO + H_2 \qquad \text{(III)}$$

$$C + 2H_2 \rightarrow CH_4 \qquad \text{(IV)}$$

$$C + \tfrac{1}{2} H_2O + \tfrac{1}{2} H_2 \rightarrow \tfrac{1}{2} CO + \tfrac{1}{2} CH_4 \qquad \text{(V)}$$

$$CO + H_2O \Leftrightarrow CO_2 + H_2 \qquad \text{(VI)}$$

giving 7 gas phase and 2 solid phase species. Species are assumed to be transported by convective and diffusive processes within each phase. Consequently individual continuum equations are solved for each species in each phase.

Reactions (I) and (II) are the exothermic coal combustion reactions which provide heat energy for the endothermic steam-char gasification reactions, (III) to (V) and the homogeneous gas-water shift reaction (VI). Reactions (I) to (V) occur between the gas and solid phase with reaction (VI) occurring only within the gas phase. All reactions may occur at any point within the flow domain, the controlling factors being local concentrations of reactants and products and temperature. Chemical reactions rates for combustion are based on experimentally derived models whilst for the gasification reactions the empirical model of Johnson (1981) is adopted. Reaction rate for the gas-water shift reaction is based on that given in Gururajan *et al.* (1992), additional details of the model are given in Witt and Perry (1995).

## 4. THREE DIMENSIONAL BUBBLE FORMATION

The first case studied consists of a vertical 300mm diameter cylinder of length 3m sitting on top of a 800mm long conical section. Fluidising air at atmospheric conditions enters the conical section of the model at two levels. At each level, three nozzles, uniformly distributed around the circumference, feed air into the conical section. To prevent solid material building up in the base of the cone a small quantity of air with a velocity of 0.1 m/s enters through the base of the cone. Air supplied to the riser through the inlets is set to give a mass flow rate of 198.7kg/hr which corresponds to a superficial riser velocity of 0.58m/s. A pressure boundary is used at the top of the riser. Solid phase density is 282kg/m$^3$, with a particle diameter of 1.1mm and a sphericity factor of 0.69. To account for viscous effects, a value of 1.0 Pa-s based on published experimental values is used for the solid phase viscosity and $1.82 \times 10^{-5}$ Pa-s for the gas phase viscosity. Initially the system is partly filled with solid phase material at a solid's volume fraction of 0.53 giving a total solids inventory of 14.48kg.

To avoid numerical problems arising from non-orthogonal cells and potential problems arising from the use of an axis of symmetry, a "five-block" pipe grid is used. Grid sensitivity of the calculation is assessed by performing a coarse and fine mesh calculation. In the coarse mesh calculation a total of 5712 cells are used. Whilst 26208 cells are used in the fine mesh calculation. Approximate CPU time for half a second of real time is 25 hrs for the coarse mesh model on a 55MHz SUN SPARC 10 and 55hrs for the fine mesh calculation on a 90MHz SUN SPARC 10.

Results for the coarse mesh model are presented in Witt and Perry (1994). Results obtained for two seconds of real time for the fine mesh model are presented in the form of gas phase iso-contours in Fig 1. Note that for visualisation purposes the vertical dimension is scaled by a factor of one half relative to the horizontal dimensions. At 0.05 seconds, the location of the six gas jets are visible as small bubbles form. The bed surface is shown as the elliptical shape part way up the plot due to the three dimensional visualisation and with time is seen to expand upward as gas enters the bed. By 0.8 seconds the six air jets have coalesced into a long single void which travels upward and breaks through the bed surface at about 1.3 seconds. Gas in the void leaves the bed 1.5 seconds. By 2.0 seconds the initial void has left the bed but solid material entrained in its wake is seen to be carried into the freeboard region. Further calculation predicts the formation of long central voids similar to the initial void shown here. A few small voids are predicted to occur near the walls, but most gas travels through the central region. Such a prediction suggests that experimental techniques based solely on inspection of the outside of clear walled systems will be of limited use for gaining an understanding of gas flow within such systems.

Results in Fig 1, when compared to earlier coarse mesh results, show that refining the grid has a small effect on the solution and hence the solution is not fully grid independent. However the main features of the flow are captured in both models with the fine mesh model showing sharper bubble definition and earlier coalescence of the air jets into a single central gas void. Expansion of the bed surface, the bubble breaking through the bed surface and the solid entrainment in the wake region are all consistently predicted by both models.

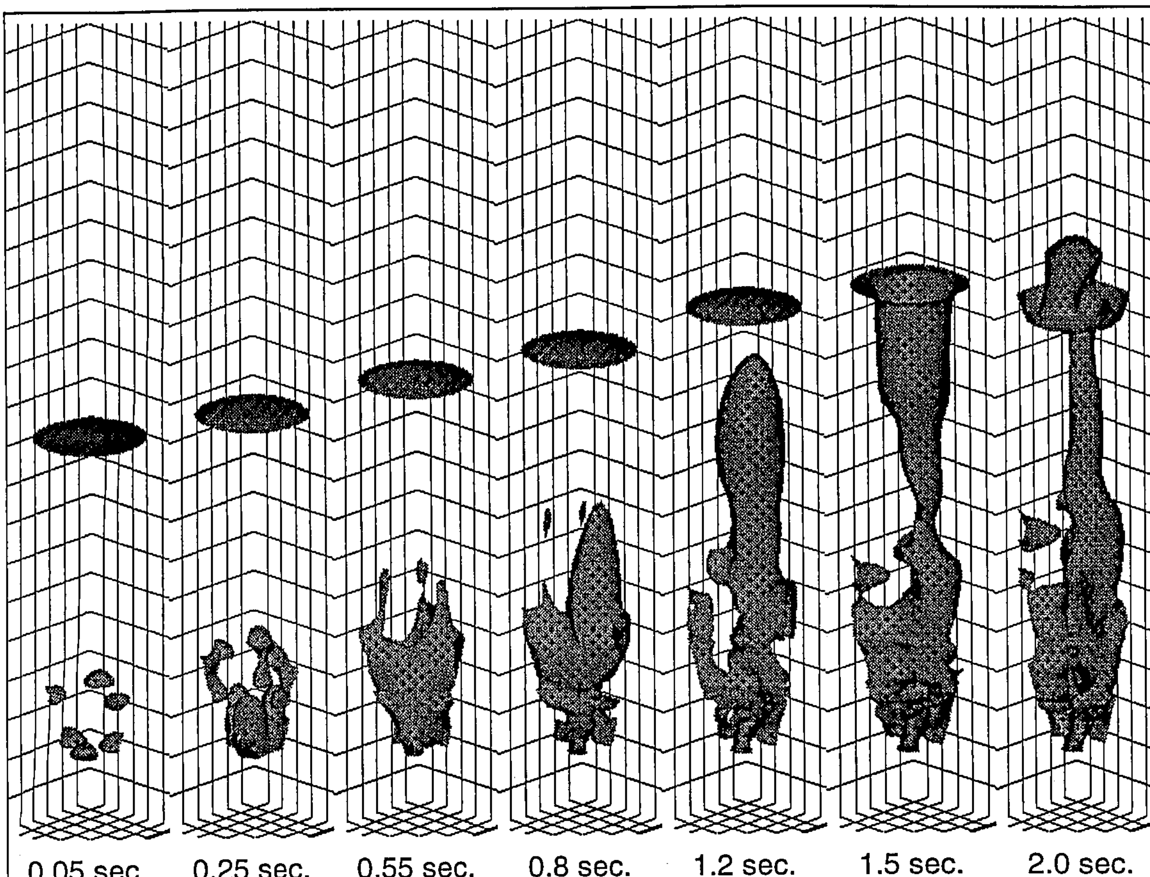


**Fig 1.** Iso-contours Showing Bubble Formation between 0.05 and 2.0 seconds with a Fine Mesh (0.8 gas volume fraction)

Recently Mathers and Rhodes (1996), using a capacitance tomographic imaging system in a fluidised bed with a similar physical geometry to that of the present model, obtained transient radial gas voidage distributions at a location 640mm above the junction of the cone and the riser. Material and thus operating conditions of Mathers and Rhodes (1996) vary from the current model and thus prevent a quantitative comparison however qualitatively the results support the model predictions. At air velocities near the minimum fluidisation velocity an almost uniform distribution was observed experimentally with occasional gas voids. At higher gas velocities long central gas voids form which are surrounded by solids near the walls at the minimum fluidisation voidage. Between gas voids the solids concentration in the centre of the riser increases but remains substantially below the minimum fluidisation volume fraction near the walls. Such behaviour is qualitatively consistent with predictions of the current model.

## 5. CIRCULATING FLUIDISED BED MODEL

Computational requirements of previous two and three dimensional bubbling bed models indicate that a full three dimensional simulation of a CFB would be prohibitive. To limit the required computer time a two dimensional CFB model is studied as a first step to a full three dimensional CFB simulation. Representing a CFB in two dimensions is a major simplification however other workers including Bouillard and Lyczkowski (1993) and Gidaspow and Therdthianwong (1993) report reasonable results with such an assumption. These previous CFD models of CFB systems employ rectangular grids which resulted in a poor representation of the geometry and poor grids as highlighted by Bouillard and Lyczkowski (1993). To avoid the problems of rectangular grids the body fitted grid systems in CFX is used.

The system modelled is an isothermal CFB with a riser height of over 4.0m and a diameter of 300mm. Fluidising air enters the riser through four air jets in a cone fitted to the base of the riser. Air jet velocities is 4m/s resulting in a superficial gas riser velocity of 2.37m/s. In a three dimensional riser this velocity would correspond to a gas mass flow rate of 707kg/hr. To account for solids recirculation and avoid problems noted by past workers with boundary conditions of the solid and gas material returning to the riser the cyclone and return leg are included in the present model. The two dimensional nature of the model does not allow the centrifugal action of the cyclone to be accounted for. To assist in separation of particles and gas, the cyclone's size is increased so that it acts as a settling chamber. Outlet of the cyclone is vented to atmosphere with both solids and air permitted to leave. However no solids are observed to leave because solid material enters horizontally and having greater momentum than the gas it tends to separate. A 90mm diameter return leg is fitted to the cyclone's base which returns solid material from the cyclone into the lower portion of the riser via a loop seal arrangement. To fluidise the loop seal a small portion of air at the minimum fluidisation velocity enter through the horizontal base of the loop seal.

Gas phase properties used in the model are those for air at ambient conditions (density 1.17 $kg/m^3$, viscosity $1.8x10^{-5}$Pa-s). Solid material used in the physical rig, upon which the numerical model is based, was crushed cork of diameter 1.1mm. Density for the cork is taken as 300kg/m$^3$. To avoid the added numerical problems and computational time required to solve a kinetic theory model to obtain solid viscosity values, a fixed solid viscosity value is adopted for the current model. A value of 1.0 Pa-s is used in the current model and is of the order of magnitude of measured and calculated values in previously published fluidised bed systems.

At walls, non-slip, partial-slip and free-slip solid velocity conditions have been used by previous modellers. Insufficient numerical and experimental work has been undertaken to show any boundary condition as being superior with all capable of predicting clusters. Experimental work by Miller and Gidaspow (1992) suggest that either non-slip or partial-slip boundary conditions would account for experimentally measured shear stresses near walls. In the present model, all walls are set to non-slip velocity conditions for both the gas and solid velocities.

A total of 9.5 seconds of real time is modelled. Solids distribution predicted by the model in 0.5 seconds intervals for the time period 7.5 to 8.5 seconds is presented in Fig 2 and shows the typical behaviour predicted by the model. Radial profiles of time averaged gas and solid vertical velocities and volume fraction are presented in Fig 3 at locations 3 and 5m above the base of the cone. To avoid the initial startup period, time averaging is performed over the last five seconds of the simulation.

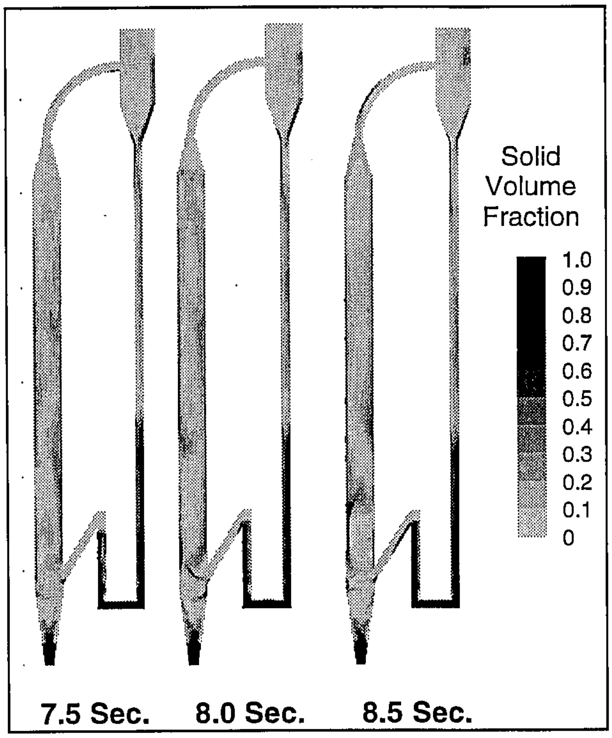


**Fig 2.** Solids Distribution for CFB Model

Results in Fig 2 show that in the riser a central upward moving region with low solid concentrations occurs whilst high solids concentrations are predicted near the walls. Solids near the walls tend to collect and form clusters typically observed in CFB systems. Not all the solids entrained in the riser separate towards the walls. Some solid material is carried over into the cyclone and can be seen to return to the base of the riser via the return leg and loop seal. In the loop seal, a bed is found to form with bubbles occurring on the inside edges of the vertical sections.

The radial profiles presented in Fig 3 at a height of 3 metres show a typical core-annular flow structure with a central core of gas moving upward and the down flow of solids near riser walls. This behaviour is consistent with that observed experimentally by Miller and Gidaspow (1992). Peak gas velocity in the riser ranges from 1.4 to 2.2 times the superficial gas velocity and agrees with the observation of Miller and Gidaspow (1992) that core gas velocities can be up to twice the superficial velocity. At 5 metres the solid concentrations near the walls and centre are lower indicating that much of the solid material has separated out onto the riser walls lower down in the riser. Lower solids concentrations result in lower gas velocities and a large core region higher up in the riser.

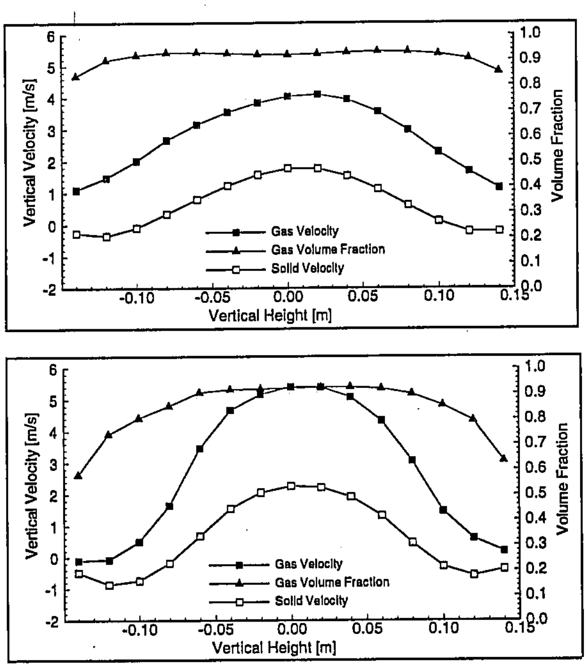


**Fig 3.** Radial Profiles of Time Averaged Vertical Velocities and Gas Volume Fraction at heights of 3m (bottom) and 5m (top).

## 6. COAL GASIFICATION

The gasification model described earlier is used to model a slugging coal gasifier. To save computation time, thus allowing more test cases to be simulated, a two dimensional model is used. The system model is based on experimental work reported by Saffer, Ocampo and Laguerie (1988) for a 180mm diameter coal gasifier. Results are obtained for seven different operating conditions.

Fig 3 shows the calculated gas temperature and volume fraction along the centre-line of the gasifier at 9.5 seconds for one operating condition. The volume fraction plot shows the presences of large gas voids with narrow regions of high solids concentrations separating the voids, thus showing the gasifier to be operating in a slugging mode as reported by Saffer *et al.* The large quantity of heat released by the combustion reactions raise the gas temperature from the inlet value of 828K to the peak temperature of 1330K just above the distributor. Gasification reactions are endothermic and absorb energy from the solid and gas phases which cause the fall in gas temperature with height. Experimental gas temperature at the outlet was 1213K which compares well with the predicted value of 1223K. Even lower values are predicted near the walls as solids concentrations at walls are higher hence greater gas production occurs and more thermal energy is absorbed.

Predicted time averaged outlet gas composition is compared in Figs 5 to 8 with results from an experimental system reported by Saffer *et al.* Model results are averaged over the period of 4.5 to 10 seconds with the first 4.5 seconds of operation being ignored.

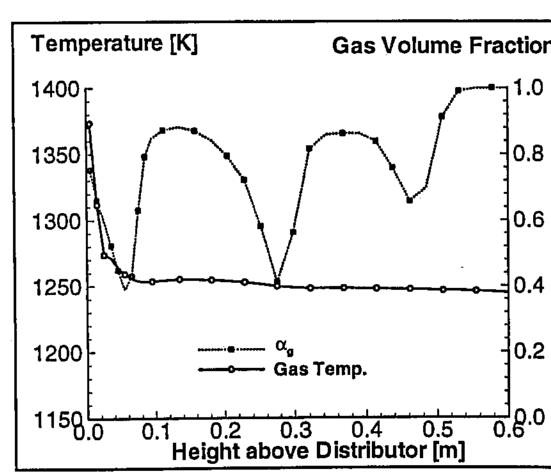


**Fig 4.** Temperature and Volume Fraction Profile along Gasifier Centre-line at 9.5 Seconds for Run 20.

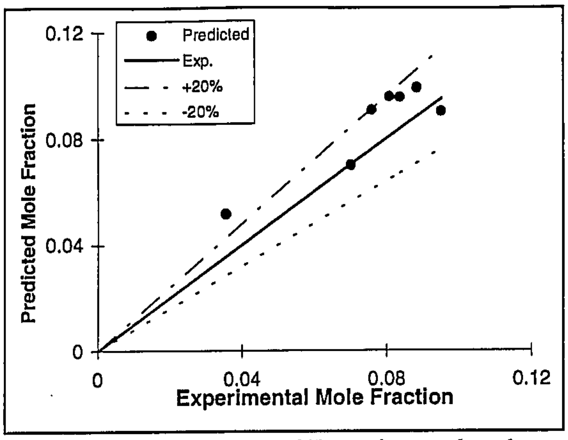


**Fig 5.** Comparison of Experimental and Predicted Average Dry $H_2$ Mole Fraction for 4.5 to 10 seconds.

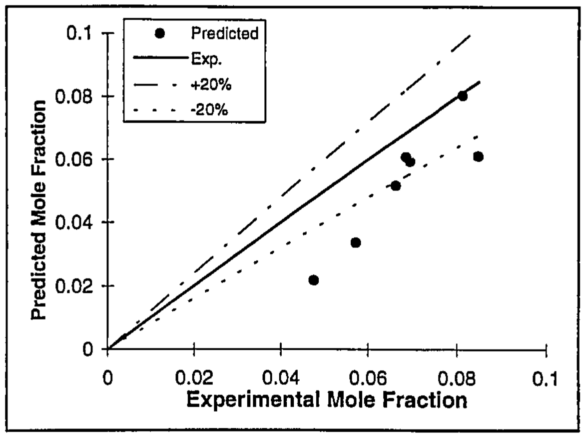


**Fig 6.** Comparison of Experimental and Predicted Average Dry CO Mole Fraction for 4.5 to 10 seconds.

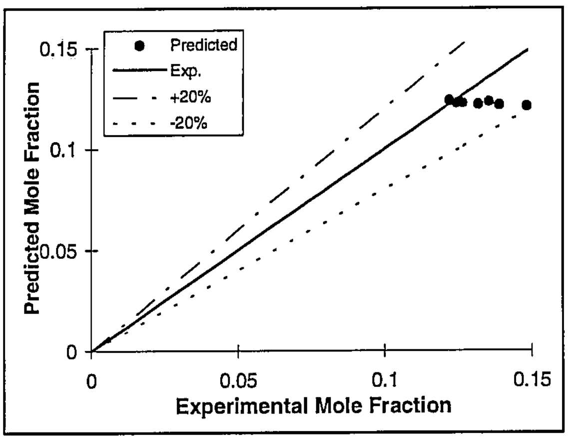


**Fig 7.** Comparison of Experimental and Predicted Average Dry $CO_2$ Mole Fraction for 4.5 to 10 seconds.

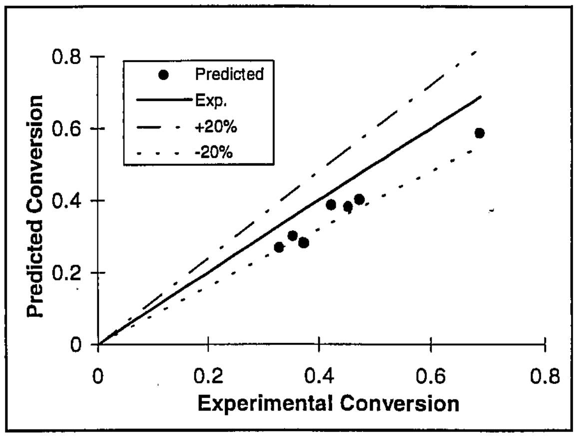


**Fig 8.** Comparison of Experimental and Predicted Average Carbon Conversion for 4.5 to 10 seconds.

In most cases predicted values fall within 20% of the experimental values and are in reasonable agreement with experiment. The exception is carbon monoxide which is consistently under predicted. Saffer *et al.* report results of their one dimensional gasifier model. Their predicted carbon conversion is closer to experimental values than that of the current model but their gas composition values are frequently in error by more than 20%. The more accurate prediction of carbon conversion is to be expected as their char reaction model is based on previous empirical data from the system. Gururajan, Agarwal and Agnew (1992) with a model using simple one dimensional hydrodynamics also simulated the gasifier of Saffer *et al.* The reaction kinetics used were similar to those used in the present model. Outlet gas properties predicted by Gururajan *et al.* are in similar agreement with experiment to those achieved by the current model. Gururajan *et al.* reports that a number of the experimental results suffer from significant mass imbalances which indicates some inconsistencies in the experimental data. Furthermore both the present model and that of Gururajan *et al.* under-predict carbon conversion by 10 to 20% suggesting that further work is required to understand the fundamental reaction processes.

## 7. CONCLUSIONS

Results presented in this paper show that CFD techniques are capable of predicting typical behaviour observed in complex fluidised bed systems. Model predictions for the different systems studied show bubble formation, the presence of clusters, a core-annular flow structure and solids recirculation. Inclusion of coal reaction rate data allows the model to be extended to predict gas composition and bed behaviour in a coal gasifier.

In most cases the lack of detailed experimental data combined with the large CPU time requirements prevent quantitative validation of model predictions. The three dimensional bubbling bed model shows that advanced experimental techniques are needed to obtain experimental data for model validation. Further work to improve confidence in CFD model predictions of complex multiphase systems is required. Such work would include collection of validation data, improvements to physical models for both gasification and hydrodynamics and means of reducing CPU time requirements of the model.


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