

# Two and Three Dimensional Simulations Investigating Dispersion and Mass Transfer Coefficients in an Eulerian-Eulerian CFD Model

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## Abstract

Eulerian-Eulerian CFD models have become widely accepted in the modeling of dense gas-solids systems. These models have been used to predicted bubble dynamics in fluidized beds and clustering and core annular structure in circulating fluidized beds. However, coupling the hydrodynamics predicted by these models with chemical reactions is relatively new application. In a recent review paper by Breault 2004 gas-solids dispersion coefficient reported in the literature differ by 5 orders of magnitude and mass transfer coefficients differ by 7 orders of magnitude. Given such variability in these coefficients this paper investigates the sensitivity of these values in the Eulerian-Eulerian model MFI (Multiphase Flow with Interphase eXchanges; [www.mfix.org](http://www.mfix.org)). Two dimensional and three dimensional simulations based on a circulating fluidized bed (CFB) in operation at the National Energy Technology Laboratory (NETL) were conducted. The simulations were conducted in the core-annular regime with carbon combustion as the single chemical reaction. The sensitivity in the predicted carbon conversion as a function of gas-solids dispersion and mass transfer coefficient is reported.

Keywords; mass-transfer, gas-solids dispersion, core-annular, CFB, eulerian

## Nomenclature

CCPI	Clean Coal Power Initiative
CFB	Circulating Fluidized Bed
$F_{gs}$	Interphase force $g/cm^3s$
$d_p$	particle diameter (microns)
$D_{O_2}$	oxygen diffusivity ( $cm^2/s$ )
$D_e$	ash layer diffusivity ( $cm^2/s$ )
$D_{mn}$	diffusion coefficient for the nth species of the gas/solids phase ( $g/cm s$ )
$\vec{g}$	force due to gravity ( $cm/s^2$ )
NETL	National Energy Technology Laboratory
$P_g$	pressure in the gas phase (Pa)
PSDF	Power Systems Development Facility
$R$	rate of production of the $n^{th}$ gas/solids

	species ( $g/cm^3s$ )
$Re$	particle Reynolds number
$\underline{\underline{S_s}}$	solids phase stress tensor (Pa)
$Sh$	Sherwood number
$Sc$	Schmidt number
$T_g$	gas temperature(K)
$T_s$	solids temperature (K)
$\vec{v}_m$	gas/solids velocity vector (cm/s)
$X_{mn}$	$n^{th}$ gas/solids species mass fraction
$X^0$	initial value of $X_{mn}$

## Greek Symbols

$\mathcal{E}_m$	gas/solids volume fraction
$\mu_g$	gas viscosity ( $g/cms$ )
$\rho_m$	gas/solids density ( $g/cm^3$ )
$\underline{\underline{\tau_g}}$	gas phase stress tensor (Pa)

## Introduction

Circulating fluidized bed technology (CFB) is being used in a variety of metallurgical, chemical and energy processes. In the energy sector, one of the promising applications of CFB's is the use of transport gasifiers in advanced coal-fueled power systems. Power plants of the future e.g., Clean Coal Power Initiative (CCPI) and FutureGen power plants will both use CFB technology to design, scale-up and operate transport gasifiers. Transport gasifiers because of their ability to operate at high throughput conditions, achieve better mixing, increase mass and heat transfer, and achieve high carbon conversion will be a key component in the overall plant design. Given such an important role these gasifiers will have on energy plants of the future, understanding the hydrodynamics and the coupling between the hydrodynamics and chemistry is critical for their design, scale-up, and operation.

To understand the hydrodynamics in a transport gasifier heavily instrumented cold flow CFB's are routinely used on a variety of scales. Experimental and

pilot scale hot units are also used to understand the chemistry and heat transfer and its dependency on the hydrodynamics. This information is obviously important, but there is no well established method for using this information for scale-up to a commercial design. Computational fluid dynamics (CFD) and Eulerian-Eulerian two-fluid models are beginning to show promise as a tool to aid engineers in the design, scale-up and operation of CFB's. There are a number of papers in the literature validating these models against cold flow units (Guenther et al. 2002, Gidaspow et al. 1992, and Tsuo and Gidaspow 1990) to name just a few. On the other hand, very little has been reported in the literature using Eulerian-Eulerian two-fluid models to simulate gas-solids systems with chemical reactions. Guenther et al. 2001 looked at the numerical effects on two and three-dimensional simulations of silane pyrolysis in a fluidized bed. Samuelbsberg 1994 considered simulations of fluidized bed reactors in his Ph.D. thesis. Recently, Guenther et al. 2003a and Guenther et al. 2003b used the two-fluid model MFIX to simulate a large pilot scale transport gasifier in operation at Power Systems Development Facility (PSDF) near Wilsonville, Alabama. This work is a joint project of the U.S. Department of Energy Southern Company Services, Inc., and Kellogg Brown & Root. These transient three-dimensional simulations considered both bituminous (Hiawatha) and sub-bituminous (PRB) coals under both air and oxygen blown conditions.

In the previous investigations done by the author simulating the transport gasifier at PSDF no effort was given to the sensitivity of the model's results on the dispersion and mass transfer models in MFIX. This paper motivated the authors, by the review done by Breault 2004, to investigate the models sensitivity in the predicted carbon conversion as a function of gas-solids dispersion and mass transfer coefficient. Two-dimensional and three-dimensional simulations of a circulating fluidized bed operating in the core-annular regime with carbon combustion as the single chemical reaction was considered. The goals of this investigation were to first understand which coefficients had a dominant effect on carbon conversion and then to run a sufficient number of simulations to correlate the predictive carbon conversion with a range of coefficient values.

### Computational Model

The MFIX model has been in use at the National Energy Technology Laboratory (NETL) for over fifteen years and has become internationally recognized as one of the premier two-fluid models available to researchers. Its open source format and FORTRAN coding of subroutines and versatile post-processing tools makes MFIX an ideal platform to develop, validate and test sub-models (e.g., dispersion and mass transfer coefficients) within a two-fluid framework. Two-fluid hydrodynamic models also referred to as Eulerian-Eulerian models, treat the fluid

and solids as two continuous and fully miscible phases. This approach results in mass, momentum, and energy balance equations for both the gas and solids phases. The continuity, momentum, and species balance equations are given below.

#### Gas-Phase Continuity

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \nabla \circ (\varepsilon_g \rho_g \vec{v}_g) = \sum_{n=1}^{N_g} R_{gn} \quad (1)$$

#### Solids-Phase Continuity

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s) + \nabla \circ (\varepsilon_s \rho_s \vec{v}_s) = \sum_{n=1}^{N_s} R_{sn} \quad (2)$$

#### Gas-Phase Momentum

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_g \rho_g \vec{v}_g) + \nabla \circ (\varepsilon_g \rho_g \vec{v}_g \vec{v}_g) = \\ - \varepsilon_g \nabla P_g + \nabla \circ \overline{\tau}_g + F_{gs}(\vec{v}_s - \vec{v}_g) + \\ \varepsilon_g \rho_g \vec{g} - R_0(\xi_0 \vec{v}_g + \overline{\xi_0} \vec{v}_s) \end{aligned} \quad (3)$$

#### Solids-Phase Momentum

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_s \rho_s \vec{v}_s) + \nabla \circ (\varepsilon_s \rho_s \vec{v}_s \vec{v}_s) = \\ - \varepsilon_s \nabla P_g + \nabla \circ \overline{S}_m - F_{gs}(\vec{v}_s - \vec{v}_g) + \\ \varepsilon_s \rho_s \vec{g} - R_0(\xi_0 \vec{v}_g + \overline{\xi_0} \vec{v}_s) \end{aligned} \quad (4)$$

#### Species Balance

$$\begin{aligned} \frac{\partial}{\partial t}(\varepsilon_m \rho_m X_{mn}) + \nabla \circ (\varepsilon_m \rho_m X_{mn} \vec{v}_m) = \\ \nabla \circ D_{mn} \nabla X_{smn} + R_{mn} \end{aligned} \quad (5)$$

where  $m = g$  or  $s$  for the gas or solids phase and  $\overline{\xi_0} = 1 - \xi_0$  and  $\xi_0 = 1$  if  $R_0 < 0$ ; else  $\xi_0 = 0$ . The eight dependent hydrodynamic variables in 3D: void fraction  $\varepsilon_g$  (the solids fraction  $\varepsilon_s = 1 - \varepsilon_g$ ), pressure  $P_g$ , and six velocity components are found by using MFIX to numerically solve the coupled non-linear partial differential equations. The number of species mass fractions ( $X_{mn}$ ) tracked are given in the chemistry model.

Constitutive relations needed to close the system, and the gas/solids energy balance equations can be found in Syamlal et al. 1993 and Syamlal 1998. A discussion on the solution procedure and further numerical references can be found in Guenther and Syamlal 2001.

### Chemistry Model

In this investigation to isolate the effects of the gas/solids dispersion and mass transfer coefficients on carbon conversion the only reaction considered in the simulations is carbon combustion given by the heterogeneous reaction  $2C + O_2 \rightarrow 2CO$ . The reaction rate is given by

$$Rate = \frac{-6\varepsilon_s P_{O_2}}{d_p \left( \frac{1}{k_f} + \frac{1}{k_a} + \frac{1}{k_r} \right)} \text{ (mol/cm}^3\text{s)} \quad (6)$$

where the film resistance is given by

$$k_f = \frac{D_{O_2} Sh}{d_p R_{O_2} T_f} \quad (7)$$

the Sherwood number is given by Gunn 1978

$$Sh = (7 - 10\varepsilon_g + 5\varepsilon_g^2)(1 + .7Re^{0.2} Sc^{1/3}) + (1.33 - 2.4\varepsilon_g + 1.2\varepsilon_g^2)Re^{0.7} Sc^{1/3} \quad (8)$$

where Re is Reynolds number based on particle diameter and the Schmidt number is given by

$$Sc = \frac{\mu_g}{\rho_g D_{O_2}}. \quad (9)$$

The ash layer resistance is given by

$$k_a = \frac{2r_d D_e}{(1 - r_d)d_p R_{O_2} T_s} \quad (10)$$

and the ratio of core diameter to particle diameter is

$$r_d = \left( \frac{X_{s,ash}^0 X_{s,carbon}}{X_{s,carbon}^0 X_{x,ash}} \right)^{1/3}. \quad (11)$$

The surface reaction is given by Desai and Wen 1978

$$k_r = 8710 \exp\left(-\frac{27000}{1.987T_s}\right) r_d^2. \quad (12)$$

### Simulation Results and Discussion

Based on the flow conditions in a large scale cold flow CFB in operation at the NETL, the initial investigation considered two-dimensional simulations of a conceptual design riser section of a CFB. The gas and solids flow rate was adjusted to produce a core-annular flow regime similar to the flow regimes found in the CFB at NETL. Core-annular flow is characterized by growth and destruction of groups of particles called clusters (Breault et al. 2005). These clusters tend to form near the walls of the riser and due to their mass can no longer be supported by the upward flow of gas fall down along the wall. Eventually these clusters break apart as they travel down and are entrained back into the upward gas flow. This constant formation and destruction of clusters produces a core-annular flow regime where near the wall (annulus) high solids concentrations and downward gas/solids velocities are found and in the center of the riser (core) low solids concentrations and high upward gas/solids velocities are found. The flow conditions are given in Table 1 and the schematic of the simulation geometry is given in Figure 1.

	Gas and Ash In	Gas and Coal In
$\rho_s, d_p$ (g/cm <sup>3</sup> , microns)	0.190, 0.9	0.190, 0.9
$\mathcal{E}_g$	0.6	0.9
$\vec{v}_g$ (cm/s)	175.0	-1.0
$X_{ash}, X_{carbon}$ (mass fraction)	1.0, 0.0	0.6, 0.4
$T_g, T_s$ (Kelvin)	1144, 1144	294, 294

Table 1. Two-Dimensional Simulation Flow Boundary Conditions

Initially the riser section was void of any solids, filled with air and at 1144K. The simulations kept the boundary conditions fixed throughout the simulation. The transient simulations were run for 70 seconds solving for the voidage, gas/solids velocity components, energy, and species mass fraction and considered only a single particle size for both the hydrodynamics and chemistry. Results were taken at the exit time averaging over the last 40 seconds of the transient data.

To investigate the values of mass transfer and gas/solids dispersion coefficients, two sets of simulations were conducted using the low (0.0005)

and high (10.0) values found in the literature for mass transfer. These mass transfer coefficients were then hard-wired into the MFIX code replacing the default model for mass transfer i.e., Gunn 1978.

Then for the low and high mass transfer numbers the gas and solids dispersion coefficients were varied to reflect the values found in the literature. The dispersion coefficients were also hard wired into the MFIX code representing a dispersive-turbulent contribution to the diffusive coefficient in equation (5). Table 2 summarized the high and low values for the gas/solids dispersion coefficients found in the literature along with the acronyms used in this paper.

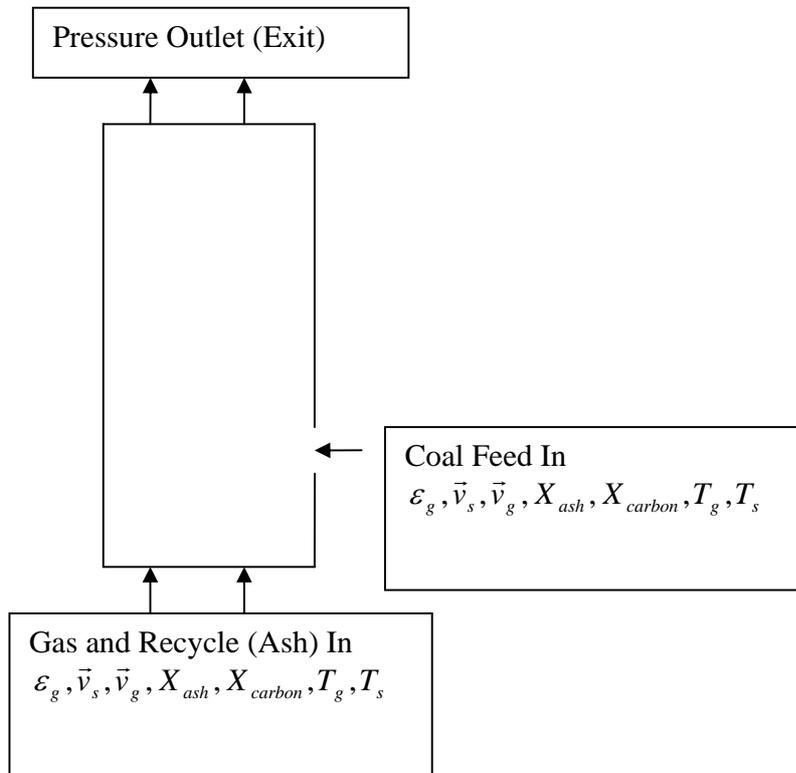


Fig. 1. Two-dimensional simulation geometry

		Dispersion Coefficients			
		High Dispersion		Low Dispersion	
		High Gas HG	High Solids HS	Low Gas LG	Low Solids LS
Gas Phase	Axial Gas	5.0		0.05	
	Radial Gas	0.05		0.0005	
Solids Phase	Axial Solids		5.0		1.0
	Radial Solids		0.5		0.08

Table 2. Low and High Values for the gas/solids Dispersion Coefficients.

Figure 2. shows the carbon conversion results for the low Sherwood number and Figure 3 shows the same results with a high Sherwood number. The vertical axis represents the percentage of carbon conversion based on the time averaged mass flow rate of carbon in the gas phase leaving the reactor. Carbon conversion is given by the following equation

$$\left(1 - \frac{\dot{M}_C^{in} - \dot{M}_C^{out}}{\dot{M}_C^{in}}\right) \times 100\% \quad (13)$$

where  $\dot{M}_C^{in}$  and  $\dot{M}_C^{out}$  are the mass flow rate of the carbon in the solids phase entering the riser (fixed boundary condition) and mass flow rate of the carbon in the gas phase exiting the reactor (time averaged).

Comparing the results presented in Figure 2 and in Figure 3, it can be seen that regardless of the value of the Sherwood number the effect of changes to the dispersion coefficients have the same trend-wise effect on the predicted carbon conversion. Comparing the cases with high gas dispersion to low gas dispersion, reveals that lower values of the gas dispersion coefficient have a significant impact on the conversion with the low value predicting carbon conversions 6 to 8 times that of the high gas dispersion coefficient. The opposite trend is observed for changes in the solids dispersion coefficient; however the magnitude of the change to the predicted carbon conversion is significantly less, being only on the order of 20 to 30 percent.

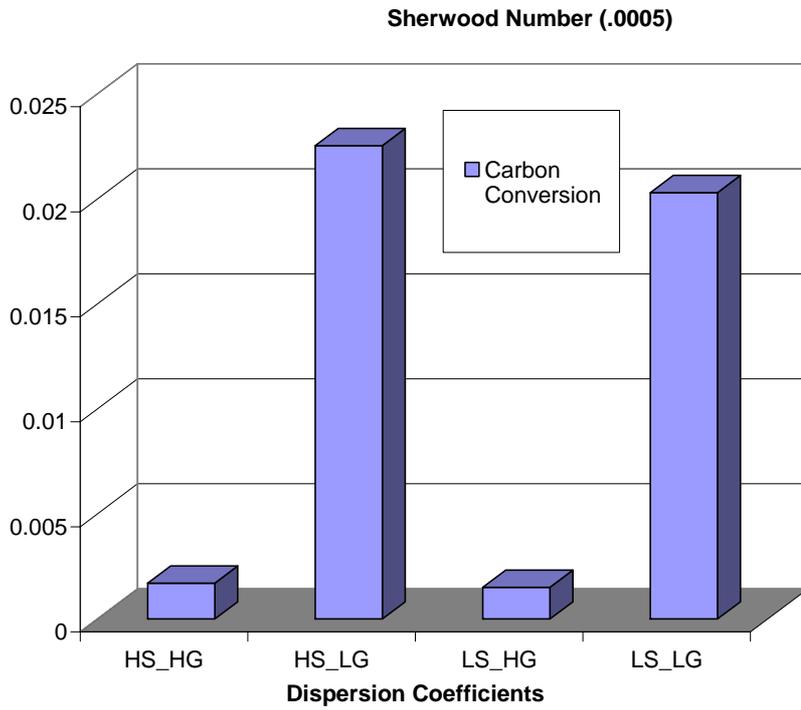


Figure 2. Carbon conversion with a low Sherwood number.

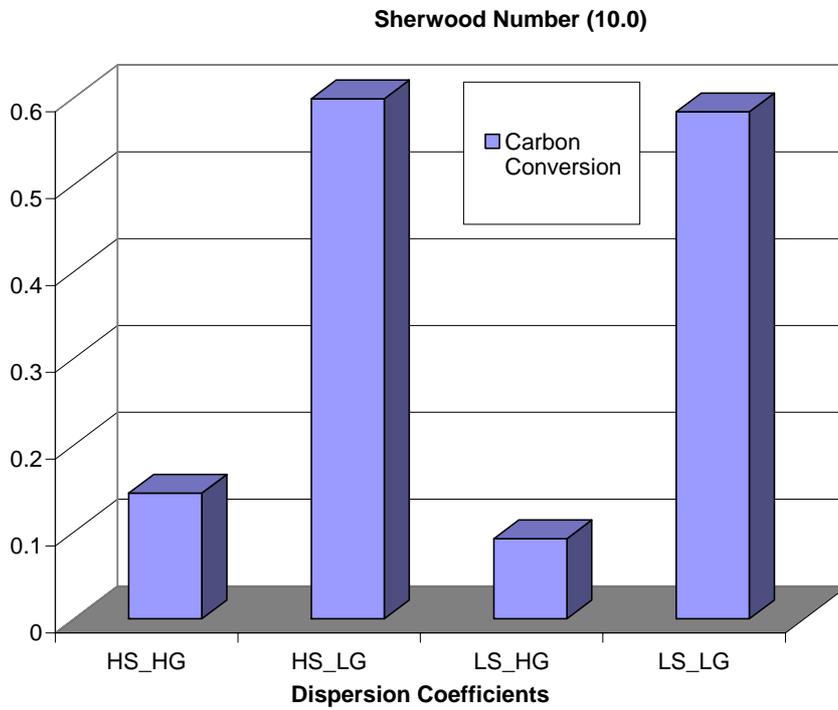


Figure 3. Carbon conversion with a high Sherwood number.

Figure 4 compares the data for high solids dispersion and high Sherwood number for several values of the gas dispersion coefficient. These being the “High Value”, the average literature value from the Breault (2004) review, the “Low Value”, and the nominal value from the MFIX default correlation. As can be seen, the carbon conversion for the average literature value falls in between the values for the “High” and “Low” gas dispersion coefficients. The carbon conversion for the prediction from the MFIX default correlation is higher than that for the “Low” case. Based upon these results, there is a strong likelihood that MFIX, for these kinetics, will over predict conversion by 25 to 30%.

To understand the sensitivity of the carbon conversion as a function of the Sherwood number simulations

were conducted using high values for the solids dispersion coefficients and low values of the gas dispersion coefficients and then varying the Sherwood number. These results are given in Figure 5. For these kinetics, carbon oxidation to CO at a nominal temperature of 1144K, the Sherwood number has very little impact on the conversion for value greater than 0.5. Recent experimental data by Breault 2005b indicates that the Sherwood number is greater than 0.5 and is approximated closely by the Gunn correlation used by MFIX.

**Sherwood Number (10.0), High Solids Dispersion**

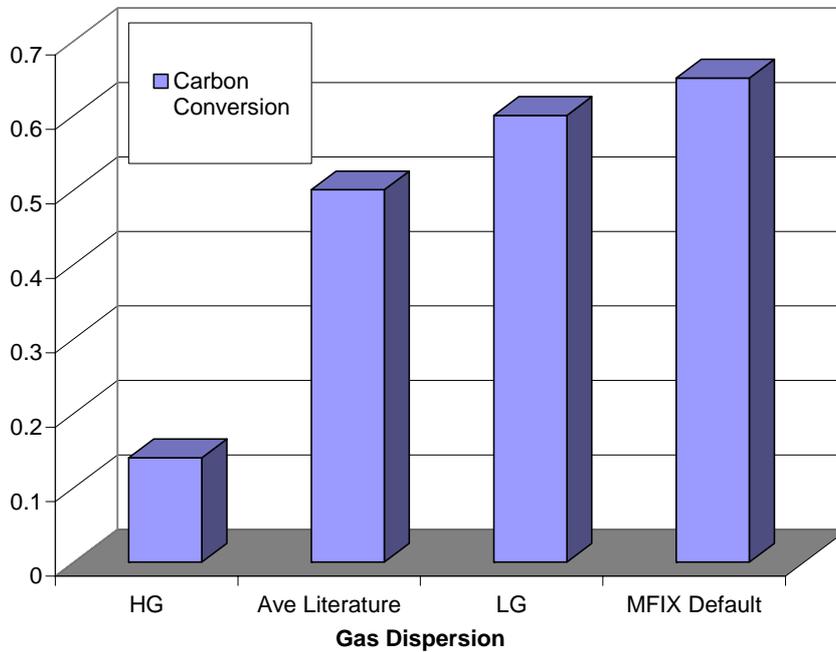


Figure 4 Carbon conversion for various gas dispersion coefficients.

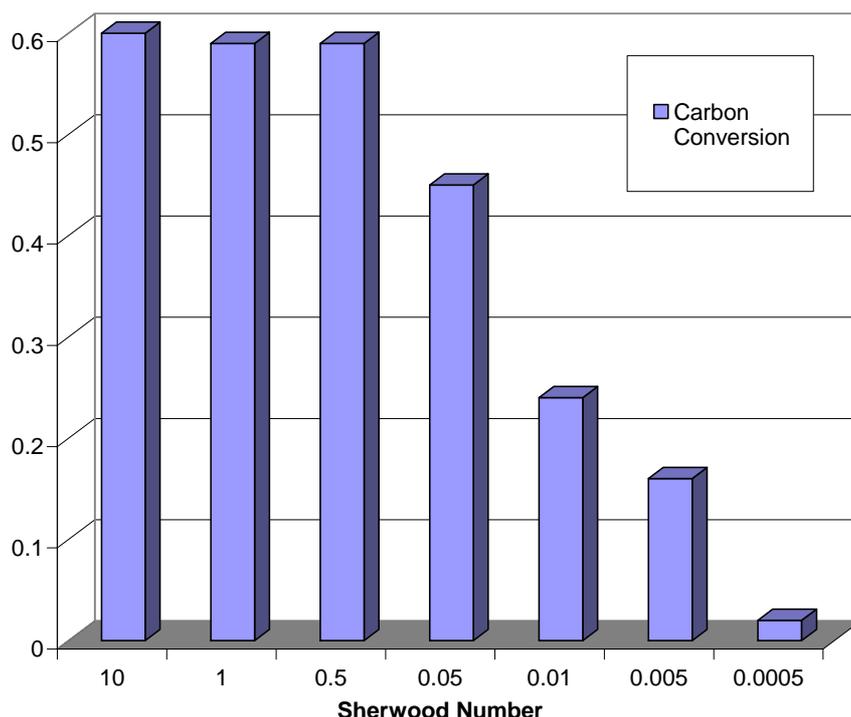


Figure 5. Carbon conversion for HS and LG as a function of the Sherwood number.

In order to determine whether the radial or axial dispersion coefficient was the dominant contribution to the carbon conversion two simulations were conducted. For these simulations the Sherwood number was determined using Gunn's expression (default in MFIX). The results given in Figures 2 and 3 showed that the gas dispersion coefficients had the dominant impact on carbon conversion and because of this the solids axial and radial dispersion coefficients were fixed at 5.0 and 0.5 respectively. The first simulation used a high axial gas dispersion coefficient of 5.0 and a low radial gas dispersion coefficient of 0.0005. The other simulation considered a low axial gas dispersion coefficient of 0.05 and a high radial gas dispersion coefficient of 0.05. The initial conditions and boundary conditions used in these simulations were identical to previous simulations reported earlier. The results showed for the high axial and low radial gas dispersion coefficients the carbon conversion was 15% and for the low axial and high radial gas dispersion coefficient simulation the carbon conversion was 52%. When comparing these values to earlier results it is clear that the sensitivity of the

carbon conversion is mainly attributed to the choice of the axial gas dispersion coefficient.

The final results presented in this paper are from three-dimensional simulations of the circulating fluidized bed in operation at NETL. Details on this unit can be found in Shadle et al. 2002. Due to the computational effort involved and the lack of available time-averaged data only preliminary results of the three-dimensional simulation are reported and work continues in this area. Figure 6 shows the mass fractions of CO as a function of height. The range of heights given in this figure corresponds to a section of the riser below and above the coal feed height. The results at each height have been spatially-averaged over the cross-sectional area of the riser and time averaged over 15 seconds of data. The results show more CO in the riser below the coal feed height for the case of high gas dispersion. High levels of CO in the low regions of a transport gasifier can inhibit the steam gasification rate. This could result in unburned carbon in the recycled material from gasifying lowering carbon conversion.

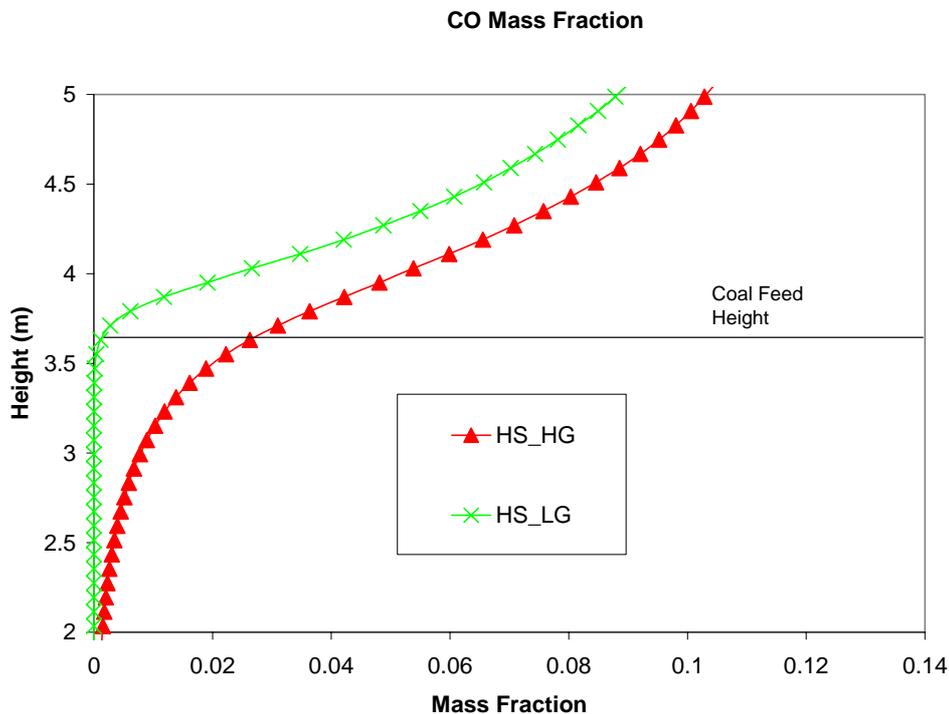


Figure 6 Mass fraction of CO near the coal feed height.

## Conclusion

Clearly, the results presented in figures 2-4 show the models predictions are sensitive to both the value of the Sherwood number and the value of the gas/solids dispersion coefficient. The results show that low gas dispersion and high solids dispersion produce the greatest carbon conversion independent of the Sherwood number. The results indicate that the gas dispersion has a dominant effect on the conversion while low or high values for the solids dispersion have secondary effects however, their effects do increase for the high Sherwood and high gas dispersion simulation. The results also show that the gas axial dispersion coefficient plays a dominant role in the

carbon conversion compared to the gas radial dispersion coefficient.

In order to evaluate the default models in MFIX (Gunn's expression for the Sherwood number, zero solids dispersion, and a gas dispersion coefficient based in part on a turbulent Schmidt number) a simulation was conducted using these default values. The values predicted for the mass transfer coefficients using Gunn's expression showed values ranging between 3.8 and 4.5, an average axial gas dispersion value of 0.00007 and an average radial dispersion value of 0.0025. With these values based on the previous results it is not surprising that MFIX predicted slightly higher conversion than the HS\_LG simulation in Figure 3.

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