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NUMERICAL INVESTIGATION OF GAS SAMPLING FROM FLUIDIZED BEDS

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NUMERICAL INVESTIGATION OF GAS SAMPLING FROM FLUIDIZED BEDS

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ABSTRACT

Gas mixing in a tall narrow fluidized bed operated in the slugging fluidization regime is studied with the aid of computational fluid dynamics. Three-dimensional numerical simulations are performed with an Eulerian-Eulerian model. Predicted axial and radial tracer concentration profiles for various operating conditions are generally in good agreement with experimental data from the literature. Different field variables including voidage, tracer concentration, and gas velocity at upstream and downstream levels are analysed to study gas mixing. Mean tracer concentrations in the dense phase and the bubble phase are evaluated and significant differences between them are found. The time-mean concentration is weighted heavily towards the dense phase concentration which may lead to misinterpretation of sampling data in dispersion models. Caution is needed when interpreting time-mean tracer concentration data. A flux-based mean tracer concentration is introduced to characterize the gas mixing in numerical simulations of two-phase fluidized beds.

INTRODUCTION

Gas mixing is an important property in gas-solid fluidized beds which significantly influences mass and heat transfer rates and plays a substantial role in determining the conversion and selectivity of chemical reactions. Therefore, knowledge of the gas mixing behavior is essential for understanding, evaluating, scaling up, and optimizing various gas-solid fluidized bed processes.

Gas mixing is usually studied by injecting tracer gas into experimental fluidized beds. Two modes of tracer-injection – transient and steady-state are common. Transient (pulse or step change) tracer injection, i.e. a stimulus-response method, is normally used to obtain the residence time distribution (RTD). This technique involves injection of a tracer into the inlet stream or at some point within the reactor and determination of the corresponding response at the exit or at some other downstream point within the reactor. For steady-state tracer studies, the tracer is injected continuously at a single or several points. Samples are then taken at different positions downstream and upstream of the injection level to obtain information on lateral/radial gas mixing. Regardless of the technique, the interpretation of experimental data is crucial to the correct understanding of gas mixing. Experimental data are often fitted to appropriate dispersion models to characterize the mixing characteristics of the system (1). However, gas sampling from fluidized beds can provide misleading information due to hydrodynamic factors, biased sampling from the dense phase, and radial gradients (2). Caution is needed to avoid these problems and to properly interpret the gas-sampling data.

The objective of this study is to explore problems that tend to occur when interpreting gas-sampling data from fluidized beds. To this end, numerical results on gas mixing in a tall narrow fluidized bed operated in the slugging regime are investigated.

NUMERICAL MODELS

3D numerical simulations were conducted based on an Eulerian-Eulerian model, with each phase treated as an interpenetrating continuum. Mass and momentum conservation equations were solved for the gas and solid (particulate) phases with appropriate closure relations. The flow was assumed to be isothermal and the gas phase incompressible. Governing equations for the solid phase were closed by Granular Kinetic Theory (3). The $k-\varepsilon$ model was employed to model the gas phase turbulence, with additional terms to account for the effect of the dispersed solid phase. The conservation equations of mass and momentum for each phase and the constitutive relations were solved using Fluent 6.3 software (4).

The numerical domain matched the experimental setup of Gilliland and Mason (5,6) who studied gas mixing in tall, narrow fluidized beds subject to steady-state tracer injection. A 76 mm I.D. cylindrical Lucite column of height 1830 mm, with a disengaging section of height 914 mm, was simulated. The cylindrical column was discretized with about 0.1 million grid points of mean grid size ~4 mm, slightly coarser in the disengaging section. Full details on the numerical models and simulation setup were provided by Li et al. (7). The particle (glass bead) properties and operating conditions are summarized in Table 1, wherever possible obtained from the experiment (8). When parameters, such as the static bed height, restitution coefficients and specularity coefficient, were not reported, reasonable values were assumed based on information in the literature. Parametric studies were also performed for these parameters as reported elsewhere (7).

Table 1. Material properties and operating conditions.

Property	Value	Property	Value
Particle diameter	155 μm	Particle density	2420 kg/m^3
Gas density	1.2 kg/m^3	Gas viscosity	1.8 $\times 10^{-5}$ Pa.s
Restitution coefficient	0.98	Specularity coefficient	0.05, 0.005
Superficial gas velocity	0.183, 0.274, 0.354 m/s	Molecular diffusion coefficient	2.88$\times 10^{-5}$ m^2/s
Particle-wall restitution coefficient	0.8	Steady state exit tracer concentration	16%, 16%, 11%
Expanded bed height	1.8 m		

At the lateral sidewall, a no-slip boundary condition was adopted for the gas phase, and a partial-slip boundary condition for the solid phase (9). At the top boundary, constant pressure was assumed, with particles free to leave the system. For the bottom distributor and the tracer flow inlet, uniform gas velocities were specified, with no particles entering the domain.

In the simulations, the bed was initially charged with stationary particles to a certain height with a solids volume fraction of 0.6. The particles were then fluidized by the primary gas flow through the bottom distributor. After fully developed flow was achieved and the bed was completely fluidized, helium was continuously injected into the system at the axis of the column through a central glass tube of 5 mm I.D. 1.05 m above the distributor to investigate the gas mixing.

RESULTS AND DISCUSSION

Among the various parameters varied in the sensitivity analyses, the specularity coefficient, ϕ, an empirical parameter characterizing particle-wall collisions in the wall boundary condition, had the greatest impact on predicted gas backmixing (7). A higher upstream tracer concentration is predicted for the low specularity coefficient for all cases simulated indicating higher backmixing. Different values of ϕ were tested in our simulations. Predicted axial concentration profiles at different radial positions and radial profiles at different levels were compared with experimental data for various superficial gas velocities and numerical predictions showed good overall agreement with available experimental data (7).

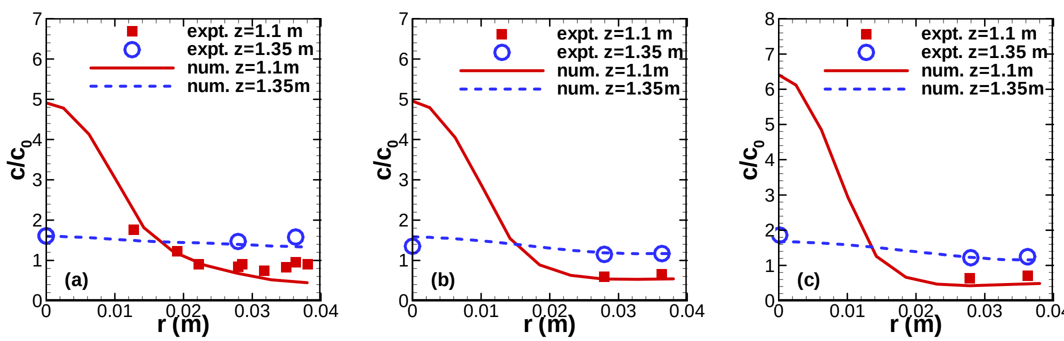


Figure 1. Radial profiles of mean tracer concentration above the injection level for U_g = (a) 0.183 m/s; (b) 0.274 m/s; (c) 0.354 m/s and experimental data from (9).

Gas sampling studies

Figure 1 shows the radial profiles of mean tracer concentration at different downstream levels. In this figure, the local mean tracer concentration, c, is scaled by the exit tracer concentration, c_0, defined as

$$c_0 = Q_{tracer} / Q_{gas} \tag{1}$$

where Q_{tracer} is the volumetric flow rate of tracer at the injector, and Q_{gas} is the total gas flow rate at the exit. As pointed out by Gilliland and Mason (6) and Grace et al. (2), the different tracer concentrations in the bubble phase and the dense phase can cause

c/c_0 >1 at some downstream levels in the whole cross-section as shown in Figure 1 for z = 1.35 m. Both numerical simulation predictions and experimental measurements show the same discrepancy. This violates the material balance when one interprets the experimental data with the widely-applied one-dimensional axial dispersion model.

To address this issue, time variations of tracer concentration, voidage, pressure, gas and solid velocities at several radial positions were monitored in the transient numerical simulations at nine upstream (z = 0.8 m) points labeled U1 to U9, and nine downstream (z = 1.3 m) points labeled D1 to D9. Positions and distribution of sampling points are shown schematically in Figure 2. Data were recorded at a frequency of 2500 Hz, i.e. with a time step of 4×10^{-4} s.

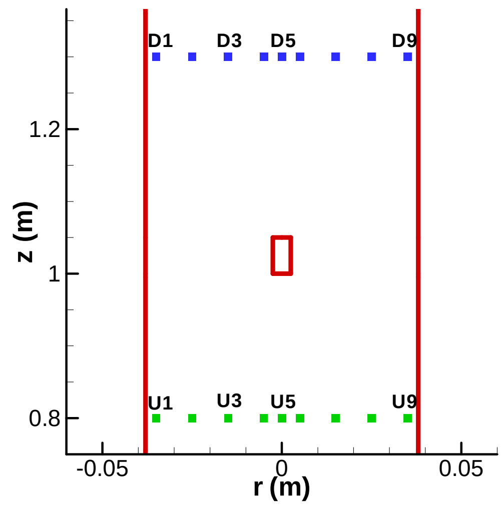
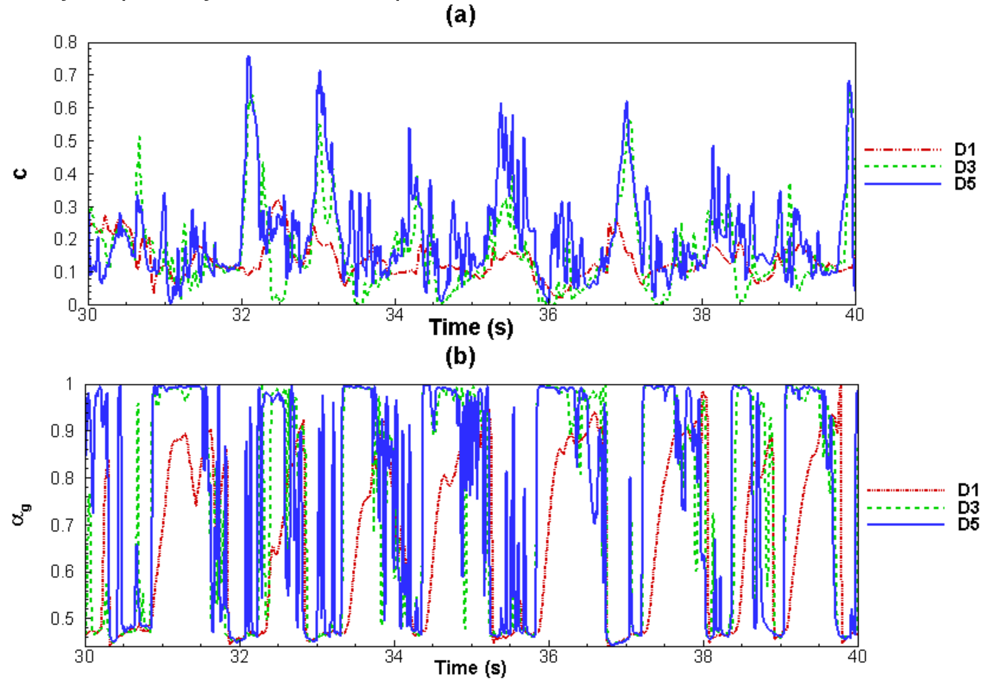


Figure 2. Schematic of positions of sampling points in the system.

Typical plots are shown in Figure 3 for the tracer concentration, voidage and vertical component of gas velocity above the injection level. For simplicity, only three positions (D1, D3, D5) are shown here. The characteristics of slug flow can be clearly observed from these plots. Downstream time variations of tracer concentration, voidage and gas velocity are very similar in the core region (D3, D5), but differ markedly from the annular region (D1). As slugs pass, substantial gas backflow is detected at D1 because of the wall effect, whereas this occurs only occasionally at D3 and is totally absent at D5 in Figure 3(c). In these plots, the tracer concentration fluctuates substantially, especially in the dense phase.



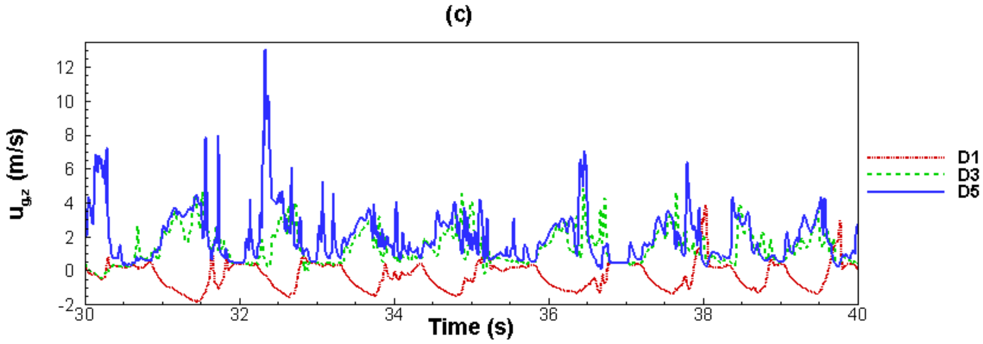
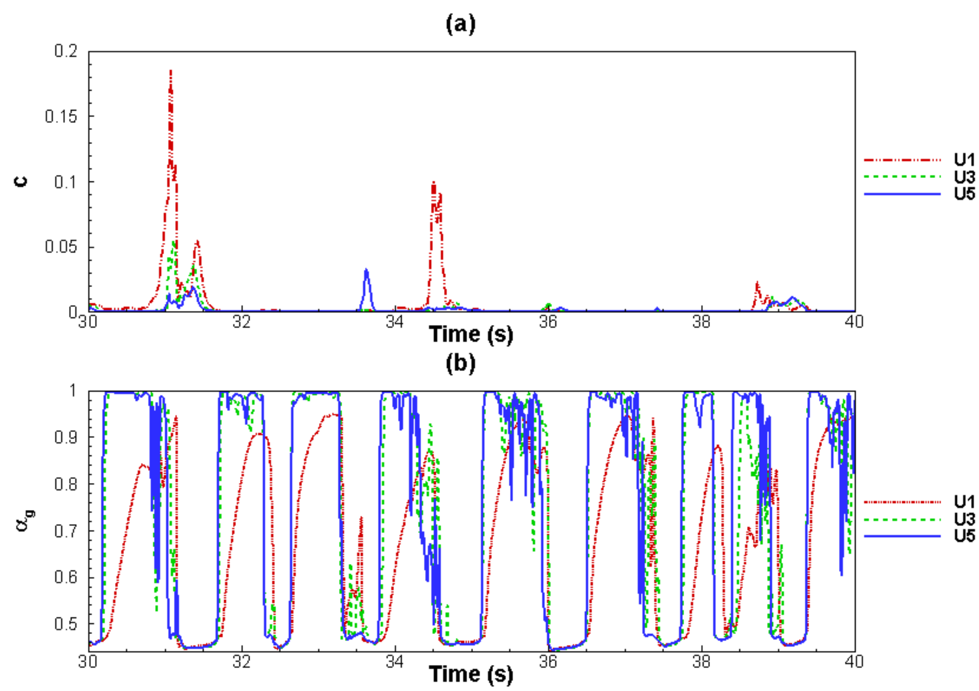


Figure 3. (a) tracer concentration, (b) voidage, and (c) gas velocity versus time at different downstream sampling points.

Similar plots at the upstream levels are presented in Figure 4. The voidage and gas velocity are similar to those in Figure 3, but the voidage pattern is more regular than downstream, especially in the central core region. The difference between the voidage at U5 and D5 indicates that some large slugs break up as they pass the injector, as observed also in the experiments (8). Only a small amount of tracer is detected occasionally upstream (below the injection level) at U1, U3, and U5. Tracer detected at U1 is carried downward by the backflow, which predominantly takes place close to the wall as slugs pass. The backmixed tracer is then gradually extracted and carried upwards by the adjacent upward gas flow. The tracer detected at U3 and U5 is mainly due to radial gas mixing from tracer transported upstream close to the wall to levels below the sampling positions.



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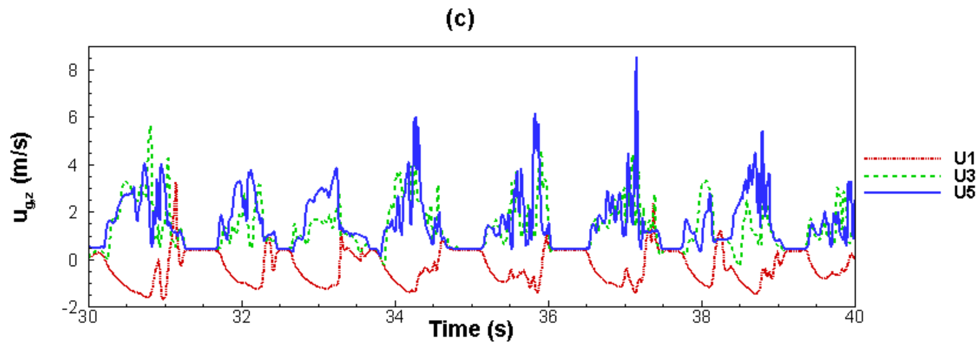

Figure 4. (a) tracer concentration, (b) voidage, and (c) gas velocity versus time at different upstream measuring points.

Note the significant difference between tracer concentrations in the dense and dilute phases. The mean tracer concentration in the dense phase and bubbles/slugs can be calculated separately by defining the bubble boundary as corresponding to a voidage of 0.8. These profiles are shown in Figure 5 along with the overall time-average concentration. It is evident that the dense phase contains higher concentrations of tracer gas than the slugs/bubbles both downstream and upstream of the injection level. Gilliland and Mason (6) noted that their continuous sampling technique tended to sample primarily from the dense phase region, and that this led to $c/c_0 > 1$ downstream of the injection level. This also occurs with the numerical simulations. As shown in Figures 3 and 4, gas in the slugs passes the sampling points at a much higher velocity than dense phase gas. Considering the high gas flux in slugs at the measuring point, the contribution of the lean phase concentration is under-estimated when the mean concentration is calculated in the time-average sense. In modelling, the time-mean concentration based on the flow through the two phases at a certain level is often used. The discrepancy between the sampled time-mean and flow-average concentrations is significant when concentrations in the two phases differ significantly (2). Failure to recognize this difference can lead to erroneous conclusions regarding both reaction progress and gas mixing. For this reason, sampling data should be interpreted with the aid of a two-phase model appropriate to the flow regime (2). In addition, the radial gradients in tracer concentration in both transient and time-average results have been demonstrated. Hence, two- or three-dimensional dispersion models are needed to properly model gas mixing.

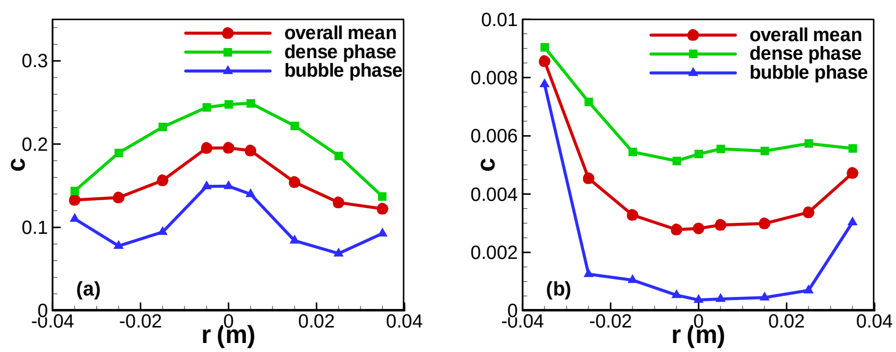

Figure 5. Profiles of mean tracer concentration and concentrations in bubble and dense phases (a) downstream (z = 1.3 m) and (b) upstream (z = 0.8 m).

With the continuing improvements in computer power and numerical algorithms, computational fluid dynamics (CFD) has become a valuable tool for studying flow in complex multiphase flow systems. It can be used to characterize mixing in place of axial dispersion models, which not only give enormous variability in fitted dispersion coefficient (10), but also lack consistency with the analogy to molecular diffusion upon which they are based (11). However, an appropriate way to interpret numerical gas sampling data is needed. Bearing in mind the bias of time-average tracer concentration toward that in the dense phase, a flux-based mean concentration similar to the flow-based mean concentration is defined to take into account the different gas fluxes in the dense and dilute phases, as follows.

$$\bar{c}_{flux} = \int_{t}^{t+\Delta t} c\varepsilon \left|u_g\right| dt \Big/ \int_{t}^{t+\Delta t} \varepsilon \left|u_g\right| dt \quad (2)$$

where ε is voidage and u_g is the gas velocity. This definition considers the two-phase nature of fluidized beds without introducing a borderline between the dense and dilute (bubble or slug) phases. The flux-based mean concentration is difficult to obtain experimentally, but it can be easily calculated in numerical simulations. The flux-based mean concentrations are plotted for the measuring points at upstream and downstream levels as shown in Figure 6. The downstream flux-based concentration is lower than c_0 (shown by a dashed horizontal line) in some regions, showing good consistency with the material balance. Upstream of the injection level, the flux-based mean concentration is also smaller than the time-average concentration, with the difference more pronounced in the central core, leading to a higher radial gradient. To some extent, this flux-based mean concentration might avoid the over-estimation of backmixing from axial-dispersion models using the time-average tracer concentration. Although further investigation is needed, the flux-based mean concentration provides a useful tool for characterizing gas mixing behaviour in CFD simulations.

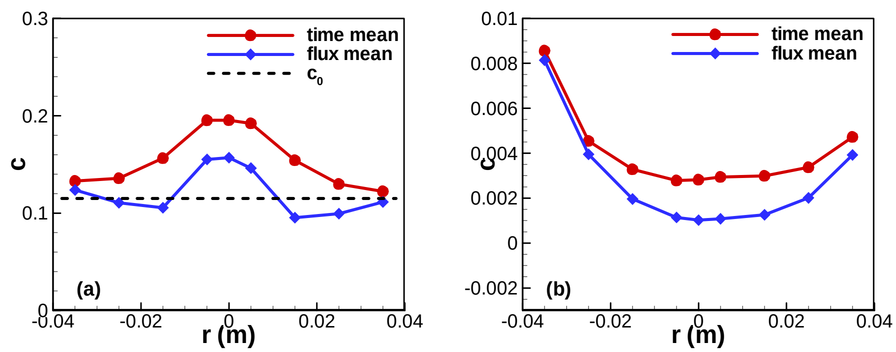

Figure 6. Flux-based mean concentration and time-average concentration (a) downstream (z = 1.3 m) and (b) upstream (z = 0.8 m).

CONCLUSIONS

Three-dimensional CFD simulations were performed to study gas mixing in a fluidized bed for which experimental data are available. Numerical results are generally in good agreement with the experimental data. Different flow field variables at the upstream and downstream levels are analyzed, and the backmixing mechanism is delineated for the slugging bed. Transient and mean tracer concentrations in the dense phase and the bubble phase show that the dense phase contains higher concentrations of tracer than the slug phase. The time-averaged local concentration is weighted towards the dense phase, which can lead to misinterpretation of experimental data in commonly-applied dispersion models. Considerable radial gradients are observed in both transient and mean tracer concentrations. To correctly interpret the sampling data, a two- or three-dimensional two-phase dispersion model appropriate to the flow regime is needed. A flux-based mean concentration is introduced which appears to be useful for characterizing gas mixing in fluidized beds and is worth further investigation.

NOTATION

c	concentration, %volume
c_0	steady exit concentration, % volume
$\bar{c}_{flux}$	flux-based mean concentration, %volume
ε	voidage, -
ϕ	specularity coefficient, -
Q_{gas}	volumetric gas flow rate, m^3/s
Q_{tracer}	volumetric tracer flow rate, m^3/s
r , z	radial and axial coordinates, m
t	time, s

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