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CFD simulations for prediction of scaling effects in pharmaceutical fluidized bed processors at three scales

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A R T I C L E   I N F O

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Experimental operation of three fluidized bed processors is compared with CFD simulation results. The capacities of the fluidized bed processors represent two orders of magnitude scale-up. Qualitative fluidization patterns as well as quantitative data are compared with simulated processor operation. The numerical method and simulation approach were found to successfully predict the flow behavior of several different sizes of fluidized beds based solely on material properties, processor loading, inlet air flow rate and fluidized bed process geometry.

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1. Introduction

Effective operation of fluidized bed processors requires a uniform gas distribution and good mixing of particles. Scaling up a fluidized bed process from lab scale to production-scale presents unique challenges such as preventing granule attrition, fines loss, or segregation. In addition, current methods make it difficult to optimize processor performance without large-scale experimentation due to the scale dependence of influences on the fluidization and related effects on the fluidized particle. Fluidization behavior is dependent on the reactor geometry and internals as well as the particle size distribution and physical properties of the powder. To accurately simulate fluidized bed behavior, it is necessary to choose a numerical method capable of accounting not only for the particle–fluid effects (e.g., drag) but also for particle–wall impacts and particle–particle interactions in three dimensions and across the entire particle size distribution.

The objective of this work was to perform a "blind test" comparison of the Barracuda® commercial computational fluid dynamics (CFD) software package from CPFD Software, LLC (Albuquerque, NM) for the modeling of fluidized bed processors. Barracuda rigorously simulates fluid–particle interactions in three-dimensions using the CPFD® numerical method by Snider [1,2] and O'Rourke et al. [3] and is an established commercial simulation software package for the study of research-scale and industrial-scale fluidized bed reactors by Zhao et al. [4], Snider et al. [5], and Parker [6]. No experimental results were shared with the CFD analyst until the simulations had been completed.

2. Experimental operation

To study the scale up effects in fluidized bed processors, particles were loaded in three fluidized bed processors of different scales. The Vector Lab Micro was operated with 150 g of solids, the Glatt GPCG-1 was operated with 2 kg of solids, and the Niro MP4 was operated with 45 kg of solids. The three fluidized bed processors and dimensions are shown in Fig. 1. The scale up from the Vector Lab Micro to the Niro MP4 represents two orders of magnitude in increased capacity.

Solid particles having a material density of 1370 kg/m^3 and a bulk density of 450 kg/m^3 were used in the experiments. The particles ranged in diameter from 2 to 1500 μm with the full cumulative particle size distribution for the particles, shown in Fig. 2. In each unit, the particle bed was fluidized with dry air at 35 °C for both a high flow case and a low flow case. Air exited through filters in the processors that prevented particles from leaving the system. All operating conditions, including inlet gas flow rates and exhaust pressure for the low and high flow cases, are shown in Table 1.

2.1. Computational method

Barracuda is a commercial computational fluid dynamics (CFD) software package from CPFD Software, LLC (Albuquerque, NM) developed for the modeling of industrial-scale particle–fluid systems. The Computational Particle Fluid Dynamics (CPFD®) method is used in Barracuda which solves the fluid and particle momentum equations

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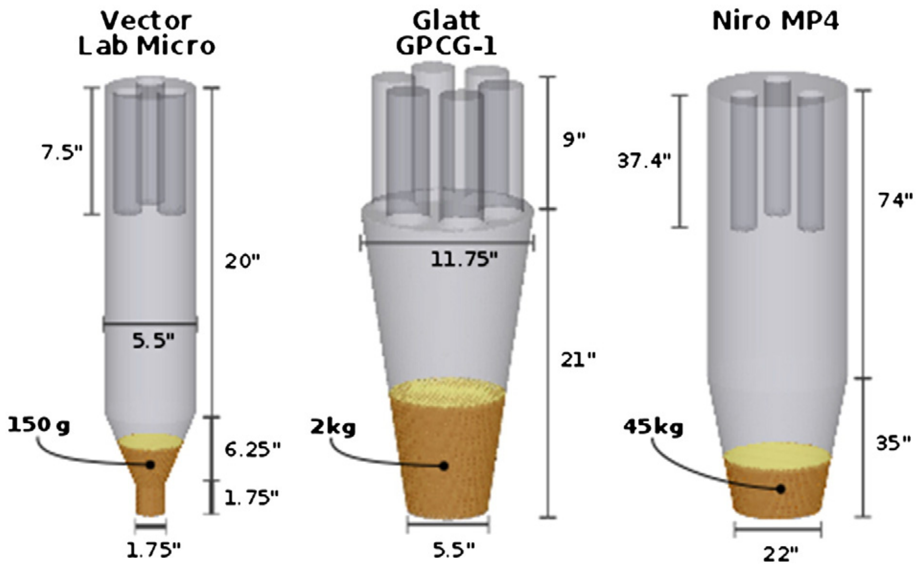

Fig. 1. Dimensions and capacity of fluidized bed processors used in the study.

in three dimensions with strong coupling between the fluid and the discrete particles. Details and development of the method are given by Snider [1,8], O'Rourke [3], and Andrews [7] and in the CPFD method, a computational particle is defined as a Lagrangian entity in which particles with the same properties such as composition, size, density, and temperature are grouped. The use of the computational particle allows large commercial systems containing billions of particles to be analyzed using millions of computational particles without losing the advantages of discretizing the solid phase in a Lagrangian frame of reference. As a result of CPFD's unique numerical approach, the following aspects of fluidized bed behavior are captured:

1. The ability to model full particle size distribution (PSD) for any number of solid species,
2. The capacity to model any solids loading from fully dilute up to close-packed (>60% solid by volume) regime in the same simulation and without prior knowledge of what the loading is likely to be,
3. Complete Lagrangian formulation for the solids, capturing mass, momentum, heat transfer, wear, etc., and
4. The ability to model systems with physical particle counts over 1E16.

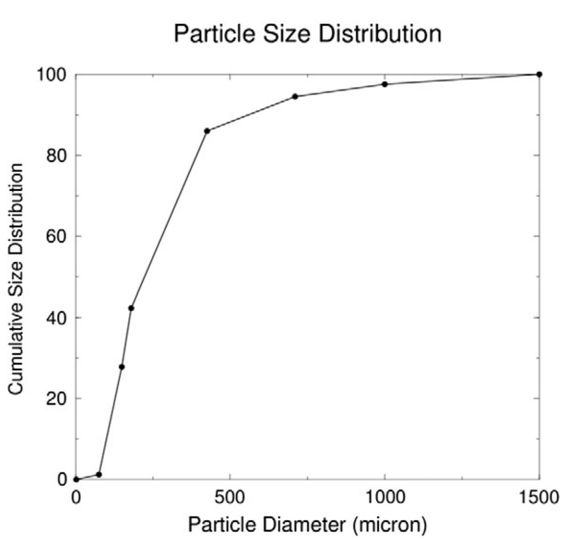

Fig. 2. Particle size distribution (PSD) of processor bed used in CFD models. The PSD is calculated by weight of the particles and was measured experimentally.

2.2. Computational model setup

Three-dimensional CFD models were created for each fluidized bed processor model. As shown in Fig. 3, the boundary conditions consisted of a uniform velocity flow boundary at the processor distributor and a pressure boundary at the processor filters. The velocity at the boundary is calculated from the distributor surface area and the flow rate listed in Table 1. The pressure boundary included a velocity dependent irrecoverable pressure drop consistent with the filter type and surface area.

Each processor operating condition was simulated isothermally at 35 °C. Particles were specified with the PSD shown in Fig. 2 and were initially at rest in the processors. For the particle information, the material density and bulk density were provided. However, in Barracuda a particle density is specified. For a porous particle, the particle density will be less than the material density. In the current work, a close pack volume fraction of 0.55 was assumed, indicating a particle density of 818 kg/m^3 and a porosity of 40%.

Each processor was modeled on a grid consisting of 50,000 to 60,000 calculation cells and 300,000 to 500,000 Lagrangian computational particles. Sixty seconds of processor operation was simulated which included fluidizing the bed from the initial resting state and steady-state operation to collect time-averaged data. Calculations were completed in 1 to 2 days for each simulation on a 3.16 GHz processor.

Table 1
Operating conditions.

	Vector Lab Micro		Glatt GPCG-1		Niro MP4	
	Low flow	High flow	Low flow	High flow	Low flow	High flow
Flow rate of air (CFM)	1.2	3.2 to 3.5	10	33	53	175
Bed mass (kg)	0.15	0.15	2.0	2.0	45	45
Exhaust pressure (kPa)	101	101	101	101	92.5	92.5
Temperature (°C)	35	35	35	35	35	35

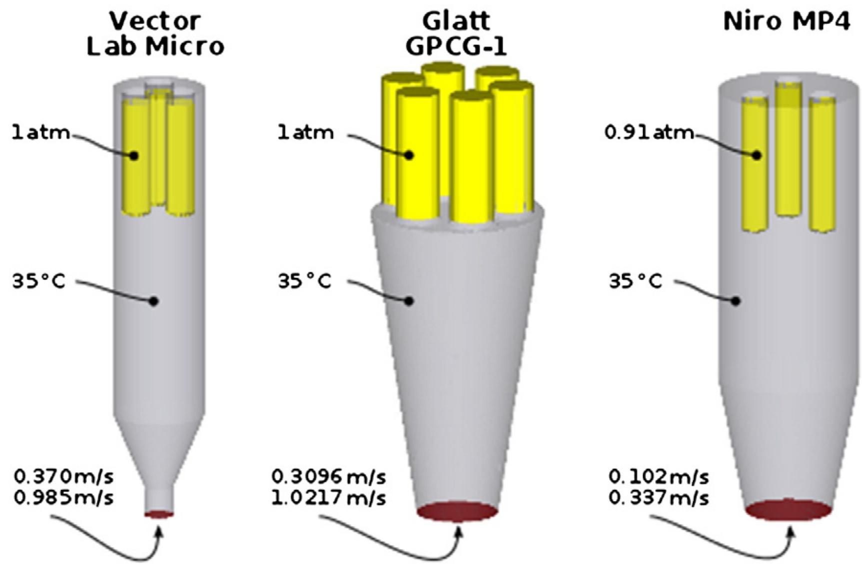

Fig. 3. Boundary conditions for CFD models of Vector Lab Micro, Glatt GPCG-1, and Niro MP4. For all models, a pressure drop existed at the pressure boundary (filters).

3. Results

The comparison between the experimental behavior and the model is based upon qualitative observations of the fluidized bed behavior, measurements of the bed height in the Vector Lab Micro and the Glatt GPCG-1, and measurements of the height to which particles were ejected into the freeboard during operation of the Vector Lab Micro.

The experimental observations of the fluidization behavior of the Vector Lab Micro are shown in Table 2. In the high flow case, it should be noted that a gas flow rate of 3.5 CFM was used experimentally whereas a gas flow rate of 3.2 CFM was simulated. A spouting bed behavior in which the height of particle ejection into the freeboard is a function of the gas flow rate was seen experimentally in both the low and high flow cases.

The spouted bed behavior observed during experimental operation was also seen in the simulation. In Fig. 4, the simulation results are shown for both the low flow and high flow cases. In both cases, the simulation shows a central jet of particles being ejected into the freeboard. The time-average volume fraction and particle mass flux indicate that the majority of particle and gas transport is occurring at the center of the fluidized bed—consistent with spouting behavior.

The experimental observations of the fluidization behavior of the Glatt GPCG-1 are shown in Table 3. At the low flow case, it was observed that the air flow was mainly through the center of the bed whereas much more complete fluidization was observed in the high flow case.

The simulation of the Glatt GPCG-1 shows that the model predicted a fluidization behavior similar to what was observed experimentally. In Fig. 5a, the solid particles are shown for the low flow case at 60 s, colored by particle volume fraction. This snapshot of the simulation shows the ejection of particles into the freeboard at the center of the bed that is typical of the low flow case. Examination of the time average volume fraction, shown in Fig. 5b, shows that on average the majority of gas flow is up the center of the bed, consistent with the experimental observation. For the high flow simulation of the Glatt GPCG-1, Fig. 5c shows significantly more particles being ejected into the freeboard and Fig. 5d shows that the gas flow is spread more uniformly through the bed than was seen for the low flow case. This energetic fluidization in the high flow case is consistent with the experimental operation.

Table 2
Experimental flow observations for Vector Lab Micro.

Low flow (1.2 CFM)	High flow (3.5 CFM)
Spouted—material reaches the cylindrical section of the bed	Spouted—material reaches about halfway between the bed surface and the filters

During operation of the Niro MP4, the sight glass unfortunately was coated in powder, making observation of the fluidization difficult. However, for the high flow case, the following was seen: "powder was being thrown about a meter above the bed. Material pressed against sight glass slowly flows downward."

Simulation results for the Niro MP4 are shown in Fig. 6. For both cases, a rolling, bubbling fluidization was observed. As shown in Fig. 6a and c, there is some material being thrown into the freeboard, however, it is difficult to fully compare the simulation results to the experimental operation of the Niro MP4.

Quantitative bed height data was collected for the experimental operation of the Vector Lab Micro and the Glatt GPCG-1 by measurement through the equipment sightglasses and transparent surfaces. Additionally, the height of the fountain inside the Vector Lab Micro was noted during operation. The fountain height is the distance that particles are ejected into the processor freeboard, measured from the top of the distributor. As shown in Fig. 7, the simulations of the fluidized bed processors compare fairly well with the quantitative experimental data. In the case of the bed height data, shown in Fig. 7a, both the experiments and simulations showed negligible expansion of the bed in the Vector Lab Micro whereas in the Glatt GPCG-1, a steady increase in bed height with air flow rate was observed in both the experiment and simulation. In the experiments with the Glatt, the bed height is consistently a few centimeters higher than expected based on the mass and bulk density however there is a fair match in the rate of bed expansion with changing air flow. As shown in Fig. 7b, the simulation of the Vector Lab Micro had a range of fountain heights that was higher than the typical experimental fountain height. It is possible that these discrepancies are due to assumptions made by the CFD analyst about the particle porosity.

4. Conclusions

The numerical method and simulation approach were found to successfully predict the flow behavior of several different sizes of

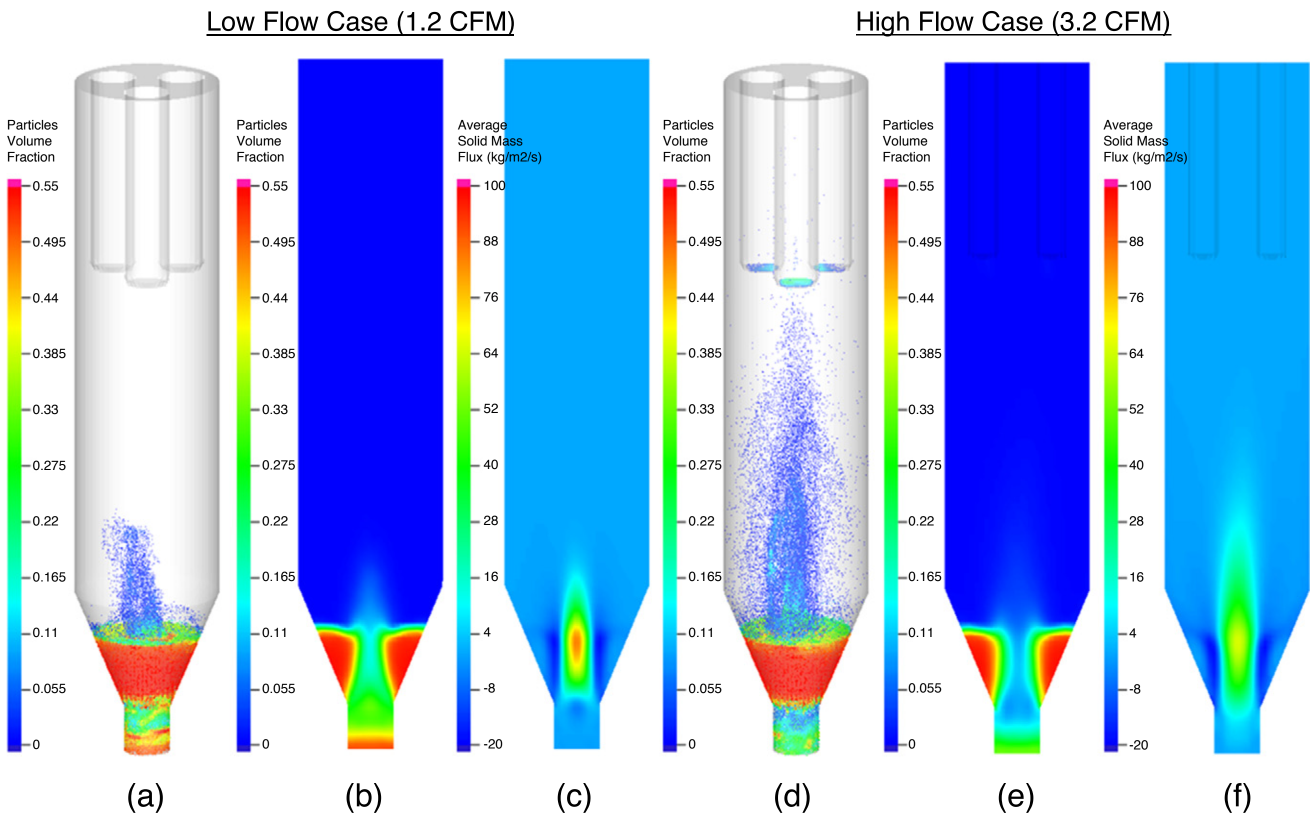

Fig. 4. Simulation results for the Vector Lab Micro model: (a and d) particles colored by volume fraction at 60 s; (b and e) time-averaged particle volume fraction at centerline; (c and f) time-averaged particle mass flux in z-direction at centerline. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 3
Experimental flow observations in Glatt GPCG-1.

Low flow (10 CFM)	High flow (33 CFM)
Flow of air is mostly in the center of the bed, material near walls is stationary	Good fluidization, bubbling throughout the bed

fluidized beds, yielding qualitatively correlated information based solely on material properties, processor loading, inlet air flow rate and fluidized bed processor geometry. The simulations modeled both start-up and steady operation of the processors on a full 3D, time-transient basis within a reasonable calculation time (1–2 days). This implies that CFD of this kind may be used to assist in determining operating parameters for fluidized bed processors commonly used in the pharmaceutical industry and in scaling processes to different sizes to meet production demands.

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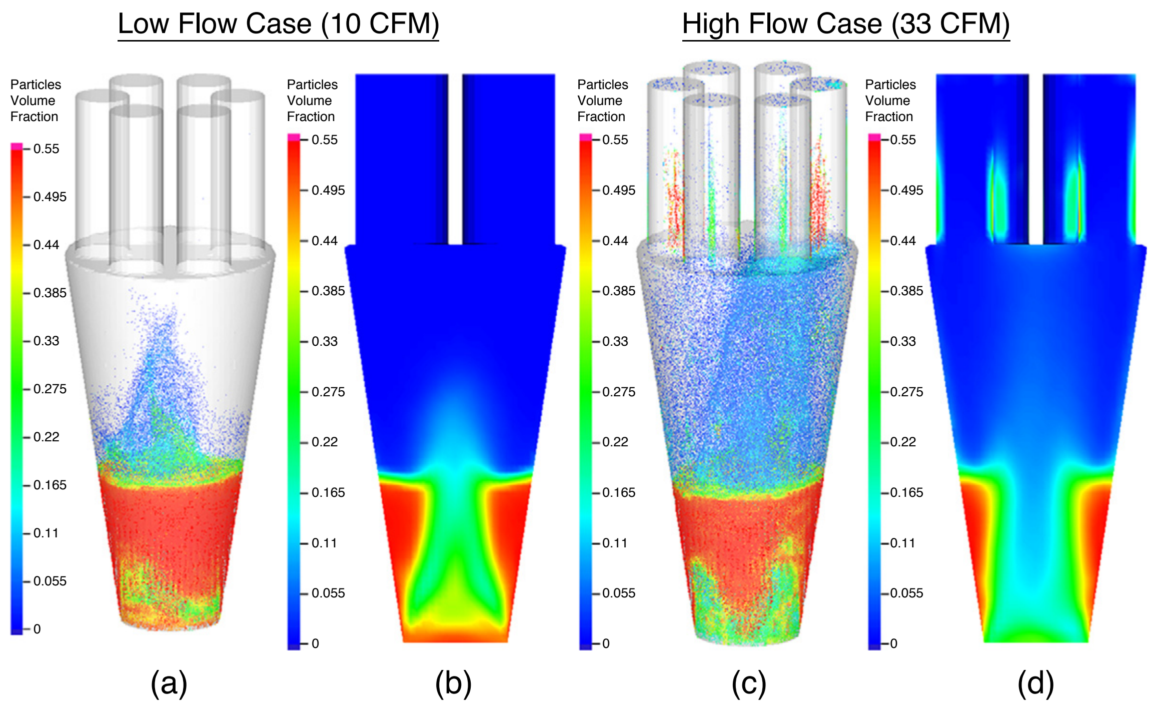

Fig. 5. Simulation results of Glatt GPCG-1 model: (a and c) particles colored by volume fraction at 60 s; (b and d) time-averaged particle volume fraction at centerline. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

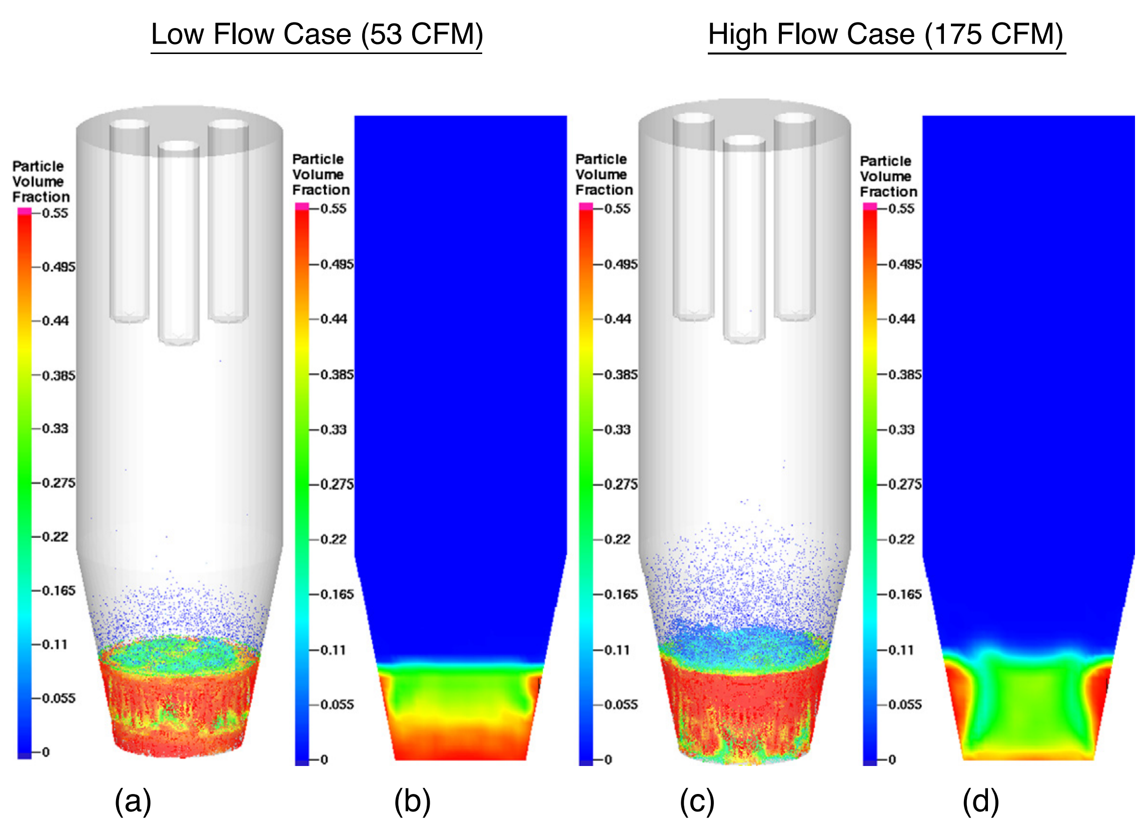

Fig. 6. Simulation results for Niro MP4 model: (a and c) particles colored by volume fraction at 60 s; (b and d) time-averaged particle volume fraction at centerline. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

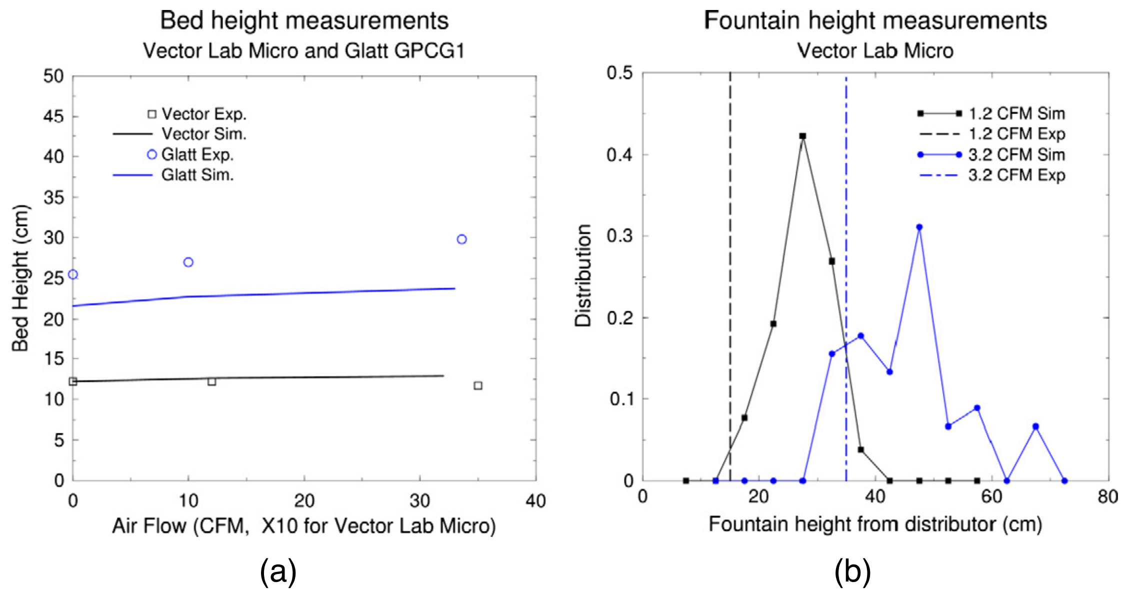

Fig. 7. (a) Bed heights in Vector Lab Micro and Glatt GPCG-1 fountain height in Vector Lab Micro; (b) comparison of typical observed height from distributor in simulation.