CONSIDERATIONS FOR PRACTICAL INDUSTRIAL CFD SIMULATIONS OF FLUIDIZED SYSTEMS

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Abstract

Computational Fluid Dynamics (CFD) is based on both fundamentals and empirical models. The fundamental principles, such as conservation of mass, momentum, and energy, are known. Empirical models, on the other hand, have more limited scopes of applicability, and thus are less understood. CFD for fluidized systems, such as fluidized beds or circulating systems, has additional inherent complexity, compared with pure fluid flows. Results can be highly dependent upon empirical models related to fluid-particle, or particle-particle interaction terms, which take the form of drag, collisional, stress, granular temperature, or similar models. The development and validation of these models, which is often undertaken at small test scales, is a topic of significant, current research. Many industrial systems utilizing fluidization, on the other hand, are constructed and operated at scales which may be orders of magnitude larger than the lab-scale or pilot-scale units upon which they are based. Industrial processes such as Fluidized Catalytic Cracking (FCC), polyolefins production, gasification, pyrolysis, or cement manufacture, to name a few, often involve characteristic length scales that can be up to ten meters or greater. This paper and presentation examine the relationship between empirical model development and practical CFD simulations of industrial systems.

Introduction

Industrial fluidization systems are at the heart of many chemical, petrochemical, and power generation processes but can be challenging to design, scale, and operate well. In recent years Computational Fluid Dynamics (CFD) models have been extended to include both particulate and fluid phases. These CFD models are based on both fundamentals and empirical models. The fundamental principles, such as conservation of mass, momentum, and energy, are known. Empirical models, on the other hand, have more limited scopes of applicability, and thus are less understood. CFD for fluidized systems, such as fluidized beds or circulating systems, has additional inherent complexity, compared with pure fluid flows. For some phenomena, results can be highly dependent upon empirical models related to fluid-particle, or particle-particle interaction terms, which take the form of drag, collisional, stress, granular temperature, or similar models.

This paper examines three case studies in which thoughtful calibration of empirical models was used to extend the validity of the overall CFD results. Practical advice is given for simulations of industrial systems.

Using U_{mf} Data to Calibrate Close-Pack Volume Fraction

In 2010, Particulate Solid Research, Inc. (PSRI) and the National Energy Technology Laboratory (NETL) released Challenge Problem III for CFD model validation. The challenge problem included two distinct systems: a circulating fluidized bed (CFB) riser experiment constructed and operated by NETL, as described by Panday et al. (2014); and a bubbling fluidized bed (BFB) constructed and operated by PSRI. For the BFB system, PSRI provided many important pieces of information about the system, including physical dimensions, static bed height, superficial gas velocity, and particle size distribution (PSD). Additionally, minimum fluidization velocity (U_{mf}) test data was provided for the particles used in the BFB, along with detailed information about the geometry and pressure tap locations in the U_{mf} experimental unit.

However, neither the close-pack volume fraction nor the apparent bulk density of the particles, from which the close-pack volume fraction could be calculated, was provided. The close-pack particle volume fraction is an important parameter in fluid-particle CFD models[1]. The particle normal stress tensor model from Snider et al. (2011), for example, ensures that particles do not exceed the physical close-pack limit observed experimentally.

The pressure drop in a U_{mf} experiment can be described by the Ergun (1952) equation. When the fluid velocity is below U_{mf}, the linear term becomes dominant, and the quadratic term is negligible. Below the minimum fluidization velocity, particle volume fraction stays constant at the close-pack value. Given experimental U_{mf} data, it is therefore possible to determine the particle close-pack volume fraction needed by a CFD model so that the measured pressure drop is reproduced. If the particles in the system are monosize, the linear term in the Ergun equation can be solved directly for volume fraction at a given fluid velocity and the corresponding measured pressure drop. However, in the PSRI BFB system, as with the most industrial fluidized bed systems, the particles have a PSD. Because the CFD model was able to account for the effects of PSD, we chose to run a series of U_{mf} simulations with different values of assumed close-pack volume fraction in order to identify the value giving the closest agreement with the initial slope of the experimental U_{mf} curves as shown in Fig. 1.

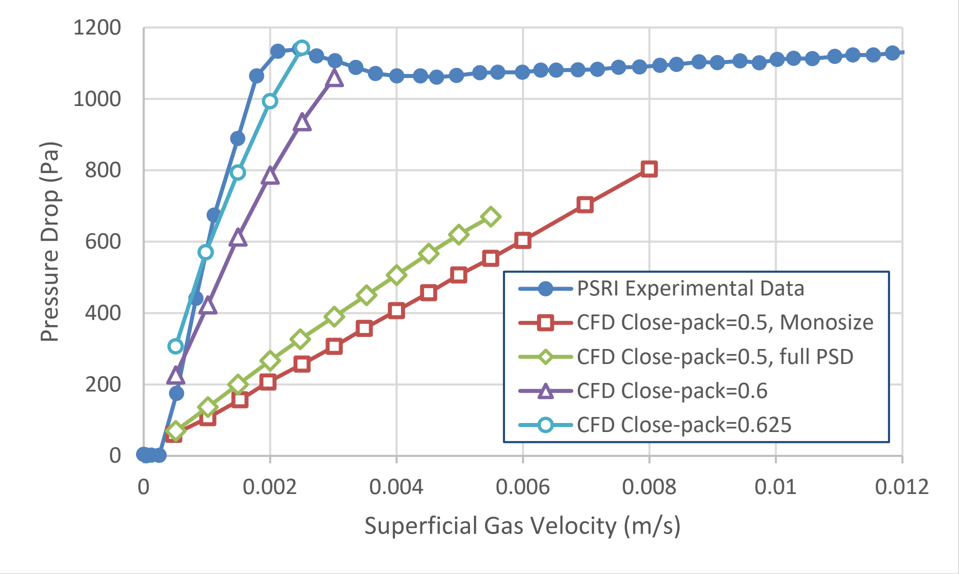

Fig. 1. Experimental U_{mf} data compared with CFD simulations using different close-pack particle volume fraction values.

Based on simulations of the U_{mf} system, we were able to identify that an appropriate value for the close-pack particle volume fraction was 0.625. Fig. 2 shows the predicted pressure profiles from two CFD simulations compared with PSRI's experimentally measured pressure profile for "Case 3" of the large-scale BFB system. The only difference between the two simulations was the close-pack particle volume fraction specified. Using a close-pack particle volume fraction of 0.5 resulted in an under-prediction of the apparent bed density in the dense bed region. By contrast, using a close-pack particle volume fraction of 0.625 raised the apparent bed density predicted by the CFD model in the dense bed region, giving much closer agreement to the experimentally measured data.

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[1] All CFD results in this paper were created using Barracuda Virtual Reactor®.

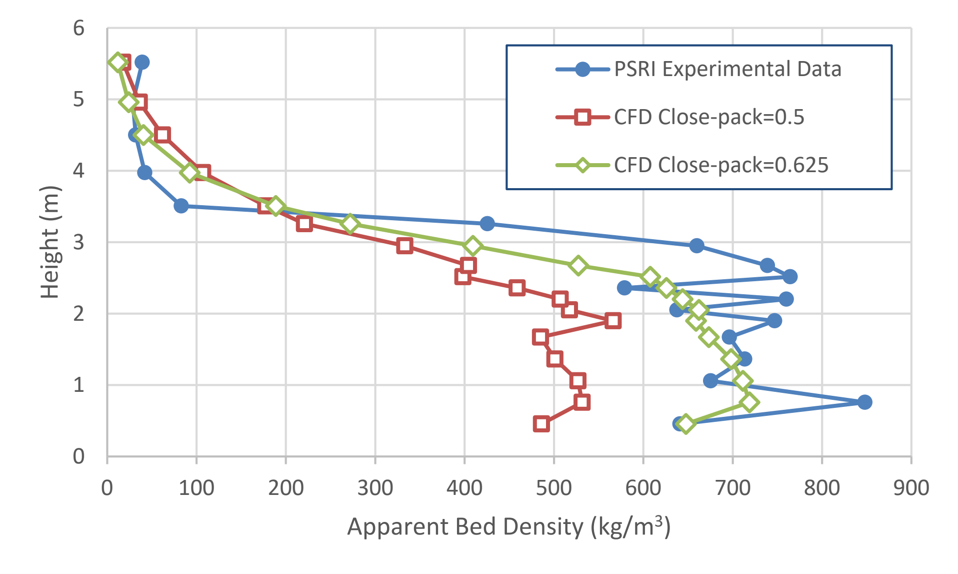


Fig. 2. Experimental apparent bed density data compared with CFD simulations using different close-pack particle volume fraction values.

Using Pressure Data to Calibrate Fluid-Particle Drag Models

Industrial fluid catalytic cracking units (FCCUs) employ fluidized bed strippers to recover hydrocarbons carried along with downward flowing spent catalyst particles from the reactor, preventing these valuable hydrocarbons from entering and combusting in the regenerator. Issangya et al. (2017) presented pressure profile results from a large-scale experiment performed by PSRI. Clark et al. (2017) presented CFD simulation results of this experimental system. The primary metric for the performance of the simulations was how well they predicted the stripper bed density as a function of gas velocity (U_g) and solids flux. Fig. 3 shows the experimentally measured data from PSRI as filled circles.

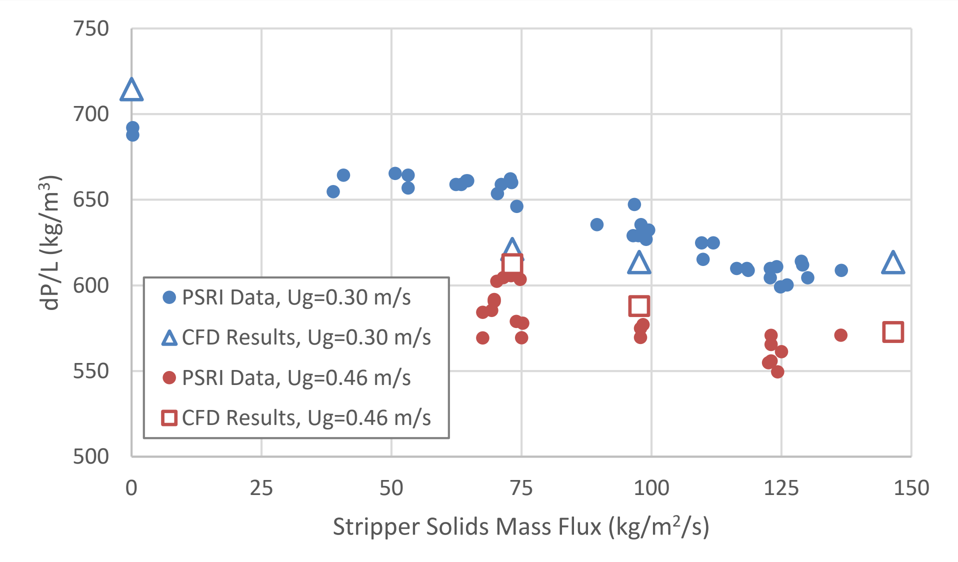


Fig. 3. Comparison of experimental data with CFD simulation results for apparent bed density

As the CFD simulation work began, the initial predictions of apparent bed density were consistently lower than the experimentally measured values. The drag model chosen for this study was a blend of the Ergun (1952) and Wen and Yu (1966) drag models, similar to the well-known blend by Gidaspow (1994). This type of blended drag model is often the first choice for simulations of fluidized bed systems because it captures different phenomena at dense loadings (for which the Ergun drag model is generally valid) and dilute loadings (where the Wen and Yu drag approaches the Shiller-Nauman correlation in the single-particle limit).

However, for simulations of Geldart Group A particles, such as the FCC catalyst used in this system, it has been observed that the Wen and Yu drag model tends to under-predict apparent bed density and over-predict particle entrainment rate from fluidized-bed systems. The authors' current best understanding of why this might happen is that CFD code implementations of drag models typically assume particles are uniformly distributed within a computational cell, and that each particle within the cell encounters the same fluid velocity. While this is generally true for homogeneously fluidized systems, as observed in liquid-solid settling experiments, such behavior does not adequately describe bubbling fluidized systems, where small-scale grouping or clustering behavior is observed.

This phenomenon of particle clustering has been a topic of significant research over the past decade, with multiple additional models proposed in an attempt to capture the missing physics. Such models, based on stable cluster size or energy minimization principles, are beyond the scope of this paper. Nonetheless, we know that some attenuation of the drag force often needs to be imposed on the Wen and Yu portion of the blended drag model so that the apparent bed density predicted by CFD models can be increased to realistic levels.

The strategy used for adjusting the drag in this study was to apply a constant multiplier, M, to the Wen and Yu portion of the blended drag model. The multiplier was also applied within the blending function to maintain a smooth transition from the Ergun drag model at higher particle volume fractions and the Wen and Yu drag model at lower particle volume fractions. To calibrate the value of M, a base case was chosen. All calibration test runs were performed on this single case, and a value of M=0.7 was found to give good agreement with the experimental data. This value was then applied consistently to all other simulations, with no further modifications to the drag model.

Fig. 3 shows the CFD simulation results compared with PSRI's experimental data. The apparent bed densities predicted by the CFD simulations captured the trends in the experimental data, and were quantitatively within the scatter of the experimental results.

Using Deaeration Data to Calibrate Particle Stress Models

An industrial example of using small-scale test data to inform empirical models used in simulations of a large-scale system was given by Loezos and Tomsula (2019). A U.S. Gulf Coast refiner was experiencing erratic stripper/standpipe catalyst circulation. Over-aeration of the standpipe was required in order to achieve stable operation of the stripper, which resulted in a low pressure build in the standpipe. A unique aspect of the operation in this unit was that the FCC equilibrium catalyst (Ecat) PSD was coarse compared with typical PSDs seen in most FCCUs.

Deaeration experiments, similar to those described by Loezos et al. (2002), were performed to measure the expansion and deaeration characteristics of Ecat with both typical and coarse PSDs. Fig. 4 shows the experimental results for bed pressure drop and bed expansion versus superficial gas velocity. The difference in fines content between the typical and coarse Ecat particles had minimal effect on the U_{mf} curve. However, it had a significant effect on the bed expansion above minimum fluidization. The sample of typical Ecat showed much greater bed expansion than the sample of coarse Ecat.

Measurements from the deaeration experiments were used to adjust the particle stress and drag models in CFD simulations of the industrial-scale stripper system, and significant differences in the particle flow behavior for the two PSDs were predicted. Fig. 5 shows particle concentration results from the CFD models at a representative instant in time. Red color indicates high particle volume fraction, and blue color represents low particle volume fraction.

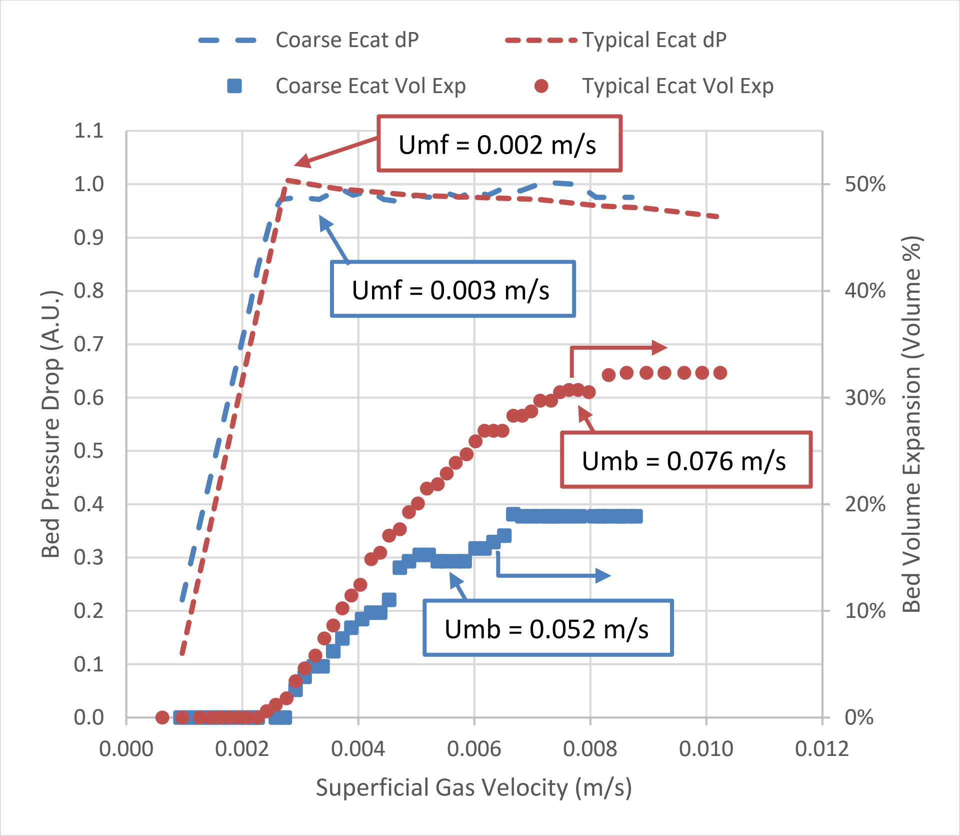
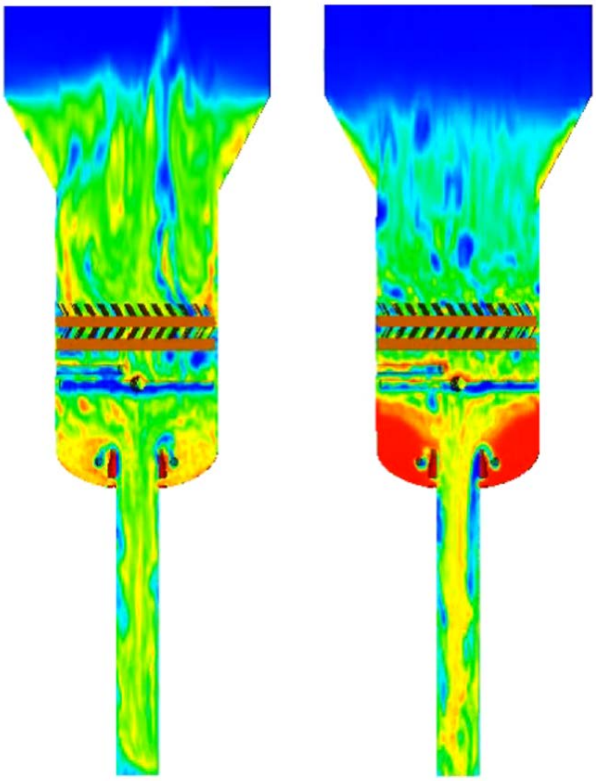


Fig. 4. Experimental data for bed pressure drop and bed volume expansion



(a) Typical Ecat **(b) Coarse Ecat**

Fig. 5. CFD Simulation results comparing particle flow of typical PSD Ecat and coarse PSD Ecat

The longer deaeration time for typical PSD Ecat allows for smoother flow through the stripper and into the standpipe. In the coarse Ecat simulation, a large defluidized catalyst zone forms in the elliptical head, extending almost all the way up to the main stripping steam ring. The fluffing steam ring cannot effectively penetrate into the defluidized zone. Additional fluffing steam, intended to fluidize the bottom of the stripper better, only acts to dilute the catalyst in the standpipe, resulting in low pressure build.

Conclusions

CFD results are partly based on empirical models, and the applicability of the output improves with model calibration. Calibration against smaller-scale test data has been shown to increase the validity of simulations and should be undertaken whenever practical. Additional calibration against operational data from the full-scale operating unit is recommended when possible. Model calibration should be targeted to the empirical models which directly relate to the phenomena of interest. Well-chosen calibration tests should be used to address specific models, preferably in isolation if practical.

CFD practitioners are encouraged to determine a reasonable set of model parameters for a system, and to avoid the temptation to tune model settings for each simulation. Models using empirical parameters which capture trends over a range of input conditions are more useful than those which require re-calibration for each case.

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