Powder Technology 254 (2014) 115–124

Contents lists available at ScienceDirect

Powder Technology

journal homepage: www.elsevier.com/locate/powtec

CFD simulations of circulating fluidized bed risers, part II, evaluation of differences between 2D and 3D simulations

Tingwen Li [a,b,*], Sreekanth Pannala [c], Mehrdad Shahnam [a]

[a] National Energy Technology Laboratory, Morgantown, WV, 26507, USA
[b] URS Corporation, Morgantown, WV 26507, USA
[c] Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

ARTICLE INFO

Available online 13 January 2014

Keywords:
Computational fluid dynamics
Numerical simulation
Circulating fluidized bed
Gas–solids flow
Riser flow
Pressure drop

ABSTRACT

Two-dimensional (2D) numerical simulations have been widely reported in the literature for qualitative, even quantitative, study of the complex gas–solids flow behavior in circulating fluidized bed (CFB) risers. It is generally acknowledged that there exist quantitative differences between 2D and three-dimensional (3D) numerical simulations. However, no detailed study evaluating such differences can be found for simulations of CFB risers. This paper presents 2D and 3D numerical simulations of three different CFB risers. Axial pressure gradients from both 2D and 3D simulations are compared with the experimental data. It has been clearly demonstrated that the 2D simulation cannot satisfactorily reproduce the 3D simulation results. A further comparison of radial profiles of void fraction and solids velocity for an axi-symmetric riser configuration is reported and the quantitative differences between 2D and 3D simulations are analyzed. In conclusion, 2D simulation is only recommended for qualitative evaluation and 3D modeling is recommended for predictive simulations.

1. Introduction

Circulating fluidized beds (CFBs) have been widely utilized in chemical, petrochemical, metallurgical, environmental, and energy industries for applications such as fossil fuel combustion, coal and biomass gasification, and fluid catalytic cracking (FCC). However, the complex gas–solids flow behavior inside CFBs coupled with the heat and mass transfer across the phases, along with chemical reactions challenges the design and operation of these industrial systems. A thorough understanding of hydrodynamics inside a CFB is needed. With the fast development of high-speed computers and computational algorithms, computational fluid dynamics (CFD) modeling has become an effective tool to improve our understanding of complex multiphase flows and it currently plays an important role in the design and optimization of industrial systems. With advanced predictive models for reacting multiphase flows, CFD can greatly accelerate the entire reactor development process with enhanced confidence levels and better performance.

One limitation of CFD modeling of CFB systems is the expensive computational cost required by the unsteady and highly coupled multi-scale characteristics of gas–solids flows. Various methods have been introduced to reduce the computational load and accelerate the simulations for gas–solids systems from both the model and computational domain perspectives as summarized in Part I [1]. One widely used assumption of CFB riser simulations is the two-dimensional flow assumption in which a cut-plane along the axis of the cylindrical column is used. A two-dimensional numerical simulation works reasonably well for a fundamental study and has wide applications for gas–solid flow study in the literature. Nowadays, three-dimensional simulations of CFB riser have become more and more affordable with the continuous advances in computational hardware. It is then of great interest to quantify the errors associated with assumptions in CFD simulations, especially the widely used 2D flow assumption.

The differences between 2D and 3D simulations of gas–solids fluidized beds have been discussed in several papers. Peirano et al. [2] compared 2D and 3D simulations of bubbling fluidized beds and concluded that 2D simulations should be used with caution and only for sensitivity analysis, whereas 3D simulations are able to reproduce both the stationary statistics and the dynamics of the system. Cammarata et al. [3] carried out both 2D and 3D CFD simulations of bubbling fluidized beds and suggested that 3D simulations should be preferable for validating the CFD models with available correlations and experimental data. Xie et al. [4] investigated the range of validity for employing simulations based on a 2D Cartesian coordinate system to approximate both cylindrical and rectangular fluidized beds. The results of three different fluidization regimes–bubbling, slugging, and turbulent–demonstrated that a

Abbreviation: 2D, two dimensional; 3D, three dimensional; CFB, circulating fluidized bed; CFD, computational fluid dynamics; DEM, discrete element method; EE, Eulerian–Eulerian; EMMS, energy minimization multi-scale; FCC, fluid catalytic cracking; HDPE, high density polyethylene; LE, Lagrangian–Eulerian; MP-PIC, Multi-Phase Particle-in-Cell; MFIX, Multiphase Flow with Interphase eXchanges; NETL, National Energy Technology Laboratory; PSRI, Particulate Solid Research Inc.; TFM, two-fluid model; UDF, User Defined Function.

* Corresponding author at: National Energy Technology Laboratory, Morgantown, WV, 26507, USA. Tel.: +1 304 285 4538.
E-mail address: tingwen.li@contr.netl.doe.gov (T. Li).

0032-5910/$ – see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.powtec.2014.01.022

2D Cartesian system can be used to successfully simulate and predict a bubbling regime where the superficial velocity is close to the minimum fluidization velocity. However, caution must be exercised when using the 2D Cartesian simulation for other fluidized regimes. A budget analysis that explains all the differences in detail was presented by Xie et al. [5] showing the role of third direction that is not resolved in 2D simulations. Reuge et al. [6] also studied the differences between 3D simulations and 2D axi-symmetric and Cartesian simulations. Their results again indicated that 3D simulations are necessary for correctly reproducing the experimental bed expansions and heights of fluctuation of a bubbling fluidized bed, while the 2D simulations widely overestimated both quantities. The 2D Cartesian calculations showed better agreement with the experiments and the 3D simulation than the 2D axi-symmetric calculations, but they still significantly overestimated the bed expansions and heights of fluctuation. Significant quantitative differences between 2D and 3D simulations on bed expansion, solids concentration, and gas and solids velocities were also reported by Li et al. [7] in a CFD study of gas mixing in fluidized beds. Similar differences in flow hydrodynamics were observed by Liu et al. [8] even though the mixing extent predicted by the 2D simulation is quantitatively similar to the 3D results. Li et al. [9] further reported that significant differences existed between 2D and 3D simulations with respect to bed expansion, bubble distribution, and void fraction and solids velocity profiles for a bubbling fluidized bed with submerged horizontal tube bundle. According to the work by Li et al. [10,11]., 2D simulation can neither be used to accurately simulate a 3D system nor a pseudo-2D system. Unfortunately, all of the above work focuses on relatively low-gas velocity fluidization regimes. Not many comparisons between 2D and 3D simulations of CFB riser can be found in the literature, despite the wide application of 2D assumptions in riser-flow simulations and the generally acknowledged limitation of 2D modeling. Li et al. [12] reported both 2D and 3D numerical simulations of a well-documented CFB riser with a square cross-section. It was found that 2D simulations under-predicted the solids inventory even with the finest grid (10-particle-diameter grid size). On the other hand, a 3D simulation with a relatively coarse grid was found to be in much better agreement with the experimental data.

The objective of this study is to document some of the differences between 2D and 3D gas–solids flow simulations so that one can adopt the best practices. In this part of the work, we focus on the differences between 2D and 3D numerical simulations of CFB riser. For this purpose, we carry out a detailed analysis of the differences between 2D and 3D simulations of CFB risers to further the investigation of Li et al. [12]. Three cases of CFB riser simulations with different system configurations and operating conditions are considered in the current study, representing a wide variety of applications. Comparison between 2D and 3D simulations, as well as available experimental data for the axial profile of the pressure gradient, is reported for each case. Further comparison of radial profiles of void fraction and solids velocity is made for a particular case. Finally, a deliberate analysis is presented to address the inherent differences between 2D and 3D simulations.

2. Numerical tests and simulation results

The numerical simulations were mainly conducted with the open-source software, Multiphase Flow with Interphase eXchanges (MFIX), developed at the National Energy Technology Laboratory (NETL). In MFIX, a multi-fluid, Eulerian–Eulerian approach is used, with each phase treated as an interpenetrating continuum. Mass and momentum conservation equations are solved for the gas and solids (particulate) phases, with appropriate closure relations [13–15]. Constitutive relations derived from granular kinetic theory are used for the solids phase. More information on MFIX, as well as detailed documentation on the model equations and the numerical implementation, can be found at the MFIX website, https://mfix.netl.doe.gov. There is an option to use the Lagrangian–Eulerian (LE) approach in MFIX [16,17], but that was not exercised in this study because with typical CFBs the LE approach is still computationally prohibitive. In addition, the commercial CFD software-ANSYS FLUENT is employed to simulate one case of gas–solids flow in an axi-symmetric riser. Similar Eulerian–Eulerian approach based on the granular kinetic theory is utilized. Detailed information on model equations solved in FLUENT can be found in the ANSYS FLUENT theory guide [18]. For all cases, both 2D and 3D simulations with identical numerical parameters and equivalent flow conditions were conducted. For brevity, additional details on numerical models as well as some grid studies are not provided here but can be found in Part I of this paper [1].

2.1. Case 1: CFB riser with a square cross-section

The first test case is based on a well-documented experiment of a circulating fluidized bed with a square cross-section as shown in Fig. 1 [19,20]. The CFB riser has a cross sectional dimension of 146 × 146 mm and total height of 9.14 m. Sand with mean diameter and density of 213 μm and 2640 kg/m^3 respectively and loosely packed bed void fraction of 0.43 is used as the bed material. In this study, a superficial gas velocity of 5.5 m/s and a solids circulating flux of 40 kg/m^{2}s are considered. As schematically shown in Fig. 2, a 2D simulation of the central symmetric plane aligned with the inlet and outlet and a full 3D simulation of the riser section are conducted with MFIX. Based on the 2D grid study reported in Part I, 2D and 3D simulations with grid resolutions of 30 × 456 and 30 × 30 × 456, respectively, are compared here. Detailed information on the numerical settings and simulation setup has been reported by Li et al. [12].

The axial pressure gradient is one of the most common measurements from experiment and based on which the axial distribution of solids is typically obtained. Furthermore, the solids inventory can be estimated through the overall pressure drop across the riser. Fig. 3 shows the axial profiles of pressure gradient predicted by 2D and 3D simulations. As shown in Fig. 3, there are significant differences between 2D

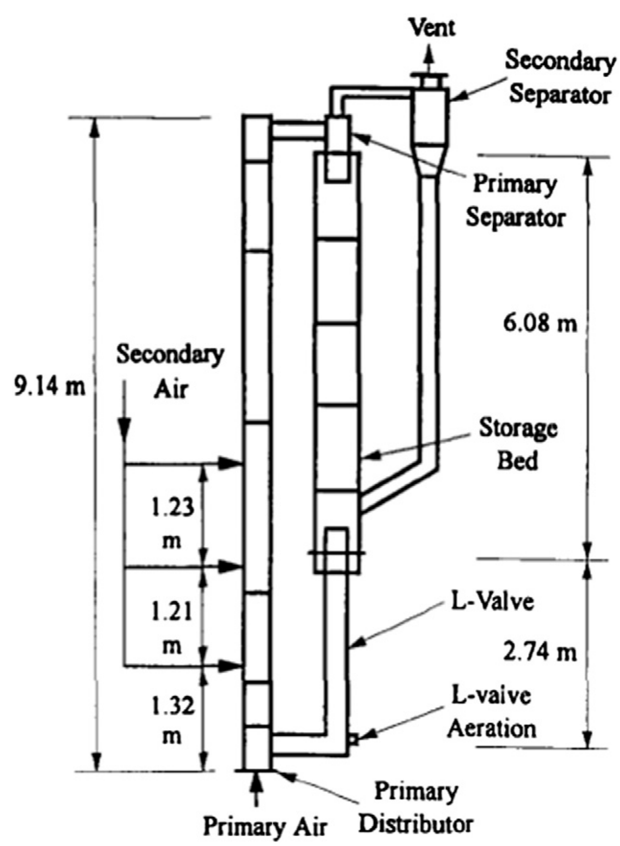

Fig. 1. Schematic of the CFB system reported by Zhou et al. [19,20].