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Representation of a small-scale nozzle for gas–liquid injections into a fluidized bed on a large-scale grid

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ABSTRACT

A novel method for efficient computations of a fluidized bed reactor with liquid injections is developed. It allows economical simulations for a reactor that contains multiple nozzles using a relatively coarse grid, while still accounting for the influence of particular features of individual nozzles. The method relies on patching variables in the near nozzle area obtained on the fine nozzle-scale grid onto the coarse reactor-scale grid followed by the solution of the flow equations elsewhere in the coarse grid domain. The procedure is tested for a small fluidized bed that permits both fine and coarse grid solutions. It was found that the developed procedure represents the flow adequately and allows for the distinction of different nozzle geometries.

1. Introduction

Liquid injections into fluidized beds take place in a variety of processes. In most cases, liquid is atomized to increase its surface area, and, hence, to improve liquid–solid contact. Quite often, the flow rate through the atomization device is limited by the spray requirements, such as droplet diameter, size distribution, and dispersion angle. Therefore, many atomizers have to be utilized in a reactor to provide the required throughput. One example of such a reactor that motivated the presented work is a Fluid Coker™ that is designed to facilitate the conversion of bitumen (a mix of heavy hydrocarbons) to lighter hydrocarbons by means of thermal cracking (Gray, 2002). The coke particles inside the reactor are sprayed by steam-atomized bitumen, which is supplied through approximately 80 specially designed nozzles. In order to obtain insight about the process, the reactor model needs to represent the complex phenomena in the reactor with sufficient accuracy to assure reasonable predictive capabilities and be practical at the same time. The objective of this work is to develop a method that will allow for the representation of the nozzles with sufficient accuracy for the reactor model to reflect the differences between different nozzle designs and parameters. This paper presents the development of the interpolation procedure.

The problem at the small-scale – a liquid injection into a fluidized bed through a single convergent–divergent nozzle – has been studied quite extensively experimentally (House, Saberian, Briens, Berruti, & Chan, 2004; McMillan, Zhou, Ariyapadi, Briens, & Berruti, 2005) as well as numerically (Pougatch, Salcudean, Chan, & Knapper, 2009; Pougatch, Salcudean, & McMillan, 2012a). Based on the known flow rates, nozzle geometry, and other process properties, the mathematical model developed by Pougatch et al. (2012a) resolves the flow through the nozzle, atomization, jet dispersion, fluidization, and droplet–particle interactions. The model can predict the velocity fields for liquid, gas, and solid phases, the average droplet diameter spatial distribution, and the liquid content of wet solid particles among other parameters. However, the model application at a larger scale that involves more than one nozzle is impractical due to rather high grid resolution requirements in the nozzle and its immediate vicinity. Therefore, there is a need for a method that would allow economical computations for a reactor that contains multiple nozzles using a relatively coarse grid while still accounting for the influence of individual nozzles.

The presence of multiple scales is very common for fluid dynamics problems. As a result, many multiscale numerical solution approaches have been developed. An extensive review of methods to address multiscale problems is presented by Ingram, Cameron, and Hangos (2004). They range from the development of submodels to approximate the equations at smaller scales (e.g. multiple turbulence models, granular kinetic theory) to non-uniform

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grids (e.g. boundary layers, jets) and to more sophisticated models that simultaneously solve appropriate flow equations at both scales with dynamic coupling (e.g. some multiphase turbulence models). An example and perspectives on the latter approach can be found in the work of Van den Akker (2010). At the same time, the multiscale character of jet injections in fluidized beds has received rather limited attention in the published literature. Either individual nozzle features were neglected as was the case in Li, Pougatch, Salcudean, and Grecov (2009) who simulated four jets injected from all sides of a rectangular fluidized bed, or the injection was limited to only one nozzle and the bed size was kept relatively small as was done by Pougatch et al. (2012a). The present work addresses the need for multiscale approach for jet injections in fluidized beds by demonstrating a fairly simple yet sufficiently accurate method of integrating nozzle and bed models.

2. Model description

2.1. General model

The mathematical model to be used for multiscale simulation has been developed by Pougatch et al. (2012a). In multi-fluid Eulerian framework, it considers turbulent flow of three phases: gas (or bubbles), liquid (or droplets), and particulate (wet or dry solid particles). Either gas or liquid can be locally continuous depending on their volume fraction values. The particulate phase is always discrete, and it consists of a solid core and a surrounding liquid layer (that can be of zero thickness for a dry particle). The size variation of bubbles (before atomization) or droplets (after atomization) is represented by an average diameter. Its variation is determined by a particle number density equation that accounts for the turbulence and drag induced bubble or droplet break-up and coalescence. The size of the dry or wet solid particles can also vary, but its variation depends only on the mass fraction of the liquid layer. The atomization is treated as a catastrophic phase inversion based only on a critical value of the gas volume fraction. It is assumed that the number of daughter droplets is equal to the number of bubbles before the inversion. Following Pougatch et al. (2009), this assumption can be illustrated by structured mesh where the bubbles are represented by cells and the droplets by nodes. All other flow properties (e.g. velocity, pressure, turbulence) remain unchanged through the phase inversion surface. Particulate phase motion is described with the kinetic theory of granular flow (Gidaspow, 1994). The model also includes mass and momentum transfer between droplets and particles to account for the inter-phase collisions resulting in rebound and coalescence. In addition, liquid that is attached to the particulate phase can also be transported during the intra-phase collisions. For reasons of brevity, the modelling equations are not presented here, but can be found in Pougatch et al. (2012a).

2.2. Multiscale solution procedure

During model application to a small-scale nozzle injection into a fluidized bed (see Pougatch et al., 2012a), it was shown that the flow in the vicinity of the nozzle exhibits little dependence of the local bed fluidization parameters, such as the superficial velocity. This is not surprising, given the high horizontal momentum that is introduced by the liquid injection. It also suggests that the nozzle scale and the bed scale can be separated. Therefore, it should be possible to solve the nozzle independently with only a piece of the fluidized bed that is representative of the bed conditions, i.e. pressure, temperature, etc. utilizing a sufficiently fine small-scale grid. Next, the obtained solution can be interpolated to a large-scale coarse grid in a manner similar to overlapping "Chimera"-type grids (Steger, Dougherty, & Benek, 1983). For all small cells that positioned inside or across the boundary of the large cell, we calculate the volume that intersects with the large cell. After that, large cell volume fractions for each phase are calculated by volume averaging:

$$\alpha_l = \frac{\sum_{\text{inside}} \alpha_s V_s + \sum_{\text{boundary}} \alpha_s V_s y_s}{V_l}, \tag{1}$$

where α is the phase volume fraction, V – the volume, and y – the volume fraction of a small cell s that lays inside a large cell l. All other variables, such as velocities, pressure, turbulence parameters, and other scalars are calculated by volume averaging using the volume fraction of the appropriate phase:

$$f_l = \frac{\sum_{\text{inside}} f_s \alpha_s V_s + \sum_{\text{boundary}} f_s \alpha_s V_s y_s}{\alpha_l V_l}, \tag{2}$$

where f represents any flow variable except phase volume fractions. Note that as the phase density is constant, the volume averaging is the same as the mass averaging. As the solution near the nozzle is practically steady-state, there is no need to repeat nozzle computations: the nozzle area can be resolved only once before the start of the large-scale simulations. During the calculations on a large-scale grid, the near nozzle cells, for which the solution was imported, have to be excluded from the computations, and the variable values in these cells have to be kept the same as the initially interpolated values. This procedure is effectively a realization of "internal boundary conditions" or immersed boundary and will result in the implicit implementation of the source terms in the equations for the computational cells neighbouring the patched variable area.[1] Definition of the so-called "frozen" or interpolation area is proven to be extremely important for successful modelling. Several trials to use cut off values based on certain flow parameters, e.g. limit the area by the velocity magnitude or the volume fraction being less that a chosen value, did not produce acceptable results and demonstrated excessive dependency on the particular test conditions. Therefore, a more general and physical procedure was developed. As the flow in the nozzle is close to axisymmetric (Pougatch et al., 2009), it will continue to be so in the jet area inside the bed as long as the horizontal momentum transferred from the jet dominates bed hydrodynamics. It means that the solution within the interpolation area has also to be axially symmetric. Moreover, any deviation from the axial symmetry takes place because of the local bed hydrodynamics of a small-scale-grid case set up and should not be exported to the large-scale solution. Doing so can introduce unphysical bias to the solution. Thus, we can determine a measure of the solution axisymmetry (x) based on the small-scale computations results and use it to define the cut off value to determine the area to be frozen on the large-scale grid. This measure should depend on a variable that is physically meaningful throughout the whole computational domain. This condition excludes liquid and particulate phases as there are areas that have either no liquid (bulk of the bed) or no solid particles (nozzle and its immediate vicinity). Therefore, we have to use a gas variable for an axisymmetry criterion. It was chosen to use the gas axial velocity variation in the azimuthal direction:

$$x = \frac{U_{\max} - U_{\min}}{U_{\text{av}}}, \tag{3}$$

where U is the velocity, and indexes max, min, and av represent maximum, minimum, and average values along the curve of constant axial and radial coordinates. In order to apply the

[1] The number of neighbouring cells would depend on the discretization scheme and the flow parameters.