A Study of the Impact of Mesh Configuration on Three-Dimensional Fluidized Bed Simulations

A Thesis Presented

by

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Abstract

The objective of this work is to study the influence of computational grid on the accuracy and efficiency of fluidized bed simulations. Due to their enhanced mixing and heat transfer characteristics, fluidized bed systems have gained attention in a wide range of industrial applications, including power generation, fuel synthesis and pharmaceuticals. Traditionally these systems are developed through extensive experimental work. Laboratory-scale prototypes often exhibit different flow characteristics than industrial-scale systems, making design and optimization even more difficult and costly. As a result, computational fluid dynamics (CFD) has become a useful tool for design and optimization of these systems. An important issue in CFD analysis of gas-solid flows in fluidized beds is the influence of mesh on the results.

The present study focuses on analyzing the reliability of fluidized bed simulations as affected by mesh configuration and resolution. Several approaches to constructing the computational grid are discussed and the influence of mesh configuration on simulation performance and accuracy is demonstrated. Given its capacity to handle both structured and unstructured grids, cases are simulated via the open-source platform OpenFOAM. The accuracy of the predictions given by OpenFOAM are validated against experimental data and compared with results from MFiX, the National Energy Technology Laboratory CFD platform. Grid resolution studies are performed, and the computational performance of various grid arrangements are evaluated.
Acknowledgements

This work would not have been possible without the support and guidance of my advisor, Professor Reza Sheikhi. I have benefitted greatly from his expertise.

Special thanks to Ronak Ghandriz, whose knowledge and assistance was integral to my efforts. Thanks also to Fatemeh Hadi and David Hensel, my colleagues in the Computational Energy and Combustion Laboratory at Northeastern University. Their collaboration and advice have made my research and studies not only possible, but far more enjoyable.

I would also like to thank Akilesh Bakshi and Christos Altantzis of the Reacting Gas Dynamics Laboratory at Massachusetts Institute of Technology, who provided much insight into the nature of this work.

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Nomenclature

Symbols

- $C_d$: Drag coefficient
- $d_p$: Particle diameter
- $e$: Restitution coefficient
- $g$: Gravitational acceleration
- $g_0$: Radial distribution
- $l$: Identity tensor
- $J_{vis}$: Dissipation due to viscosity
- $J_{turb}$: Production due to turbulence
- $K_{gs}$: Interphase drag coefficient
- $p$: Pressure
- $p_s$: Solid phase pressure
- $p_{s,kin}$: Kinetic component of solid pressure
- $p_{s,f}$: Frictional component of solid pressure
- $q_{\theta_{sw}}$: Granular energy flux at the wall
- $Re_p$: Particle Reynolds number
- $t$: Time
- $u_\varphi$: Velocity of phase $\varphi$

Subscripts, Superscripts and Other Symbols

- $g$: Fluid phase
- $s$: Solid phase
- $Q^T$: Transpose of $Q$
- $\overline{Q}$: Average of $Q$
- $\nabla \cdot Q$: Divergence of $Q$
- $\nabla Q$: Gradient of $Q$
- $Q: Q$: Double dot product

Greek Symbols

- $\alpha_\varphi$: Volume fraction of phase $\varphi$
- $\alpha_{s,max}$: Maximum solid volume fraction
- $\gamma_s$: Dissipation from interparticle collisions
- $\mu$: Dynamic viscosity
- $\rho$: Density
- $\Theta$: Granular temperature
- $\kappa_s$: Granular energy conductivity
- $\lambda_s$: Solid bulk viscosity
- $\tau$: Stress tensor
- $\varphi_f$: Angle of internal friction
- $\phi$: Specularity coefficient
1 Introduction

Due to their increased heat and mass transfer rates and their enhanced mixing characteristics, fluidized bed systems have gained interest in a variety of engineering applications, particularly in the oil and gas industry [1]. Detailed understanding of processes involved in these systems is essential for their design and performance optimization. This has proven to be a difficult and costly process, particularly for industrial- or commercial-scale systems [2]. Traditionally scale-up is done through experimentation. Computational fluid dynamics (CFD) has been widely studied as a method to supplement experimental efforts in fluidized bed design.

Even without considering heat transfer or chemical reactions, accurate simulation of multiphase flow systems, such as fluidized beds, present difficulties due to the dynamic nature of the solid-fluid interactions. There are two main approaches to multiphase flow analysis: the Eulerian-Lagrangian and Eulerian-Eulerian models. In the Eulerian-Lagrangian model, the equations of motion are solved for each solid particle as it interacts with the continuous fluid phase and surrounding particles. The ability to apply the Eulerian-Lagrangian model are limited due to the high computational cost required to compute the large number of interparticle interactions. Alternatively, the Eulerian-Eulerian model treats all solid and fluid phases as interpenetrating continua [3]. Though this enables analysis of large-scale systems, it requires complex closure models to account for particle-particle and particle-fluid interactions.

The instantaneous behavior of the flow in fluidized beds has been the subject of extensive investigation, both experimentally and using CFD. In previous studies, both two-dimensional and three-dimensional geometries have been considered. Experimentally, simulations in pseudo-2D conditions have been performed [4-6]. The front and back walls can be made transparent, which aids in optical analysis. Numerically, simulations of fluidized beds require relatively fine mesh sizes to capture the solid-fluid interactions. In addition, the unsteady nature requires a transient solver and time-averaging data over a long period to properly assess hydrodynamic characteristics. Given these factors, simulations are often performed as two-dimensional due to the reduced computational cost. Cranfield [7] and Geldart [8] observed differences in bubble characteristics between two- and three-dimensional fluidized beds. Cammarata et al. [9]
compared bubble characteristics in two- and three-dimensional simulations and found the three-dimensional case to be more realistic. Xie et al. [6,10] examined two- versus three-dimensional cases, noting that the differences between the two increases as the fluid velocity is raised. Cammarata et al. [9], Peirano et al. [11] and Xie et al. [6], [10] all conclude that the application of two-dimensional analysis must be used with caution as its accuracy is highly problem dependent. Both Bakshi et al. [12] and Verma et al. [13] simulated three-dimensional cylindrical fluidized beds and showed good agreement with experimental results. It becomes clear that conducting three-dimensional analysis provides more realistic representation of the system hydrodynamics. Furthermore as fluidized beds are most often cylindrical, an accurate numerical case should take the wall curvature into account.

The CFD platform OpenFOAM has gained much interest in recent years. OpenFOAM is a comprehensive CFD toolbox containing a multitude of built-in solvers and utilities. As it is open-source, its source code library is readily customizable, making it an attractive option for research. Numerical discretization is based on the finite volume method and allows for unstructured meshes, enabling analysis of complex geometries. OpenFOAM also shows good parallelization performance, making it suitable for use in cases with large number of grid points. In the present study the two-phase solver `twoPhaseEulerFoam`, which has developed over several years [14-18], is applied. The solver applies the Eulerian-Eulerian methodology and includes a number of closure model options common to the two-fluid method. This solver is readily applicable to a two-phase fluidized bed.

The goal of this work is to assess the impact of mesh configuration as applied to three-dimensional cylindrical fluidized beds. Due to its accommodation of unstructured meshes, OpenFOAM (version 2.3.1) [19,20] is used to implement four mesh configurations. Cases are validated against the experimental data provided by Makkawi et al. [21]. Comparison is done with the numerical results generated by Bakshi et al. [12] using the CFD platform MFiX. MFiX was developed at the National Energy Technology Laboratory, particularly for multiphase flow simulation and analysis [22-25]. It is commonly used in computational fluidized bed analysis. Once a mesh-independent solution is
obtained for each mesh arrangement, their runtimes are compared as a measure of computational performance.

2 Hydrodynamic modeling

2.1 Governing equations

In this work the Eulerian-Eulerian model is applied to simulate the conditions given by Makkawi et al. [21]. As both the solid and fluid phases are considered interpenetrating continua, the conservation equations governing a single-fluid flow can be modified to account for the solid phase. For this the concept of the phase volume fraction $\alpha_\varphi$ of phase $\varphi$ where

$$\sum_\varphi \alpha_\varphi = 1$$  \hspace{1cm} (1)

Neglecting chemical reactions and heat transfer effects, the mass conservation of the solid and fluid phases become

$$\frac{\partial (\alpha_g \rho_g u_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g u_g) = 0$$ \hspace{1cm} (2)

$$\frac{\partial (\alpha_s \rho_s u_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s u_s) = 0$$ \hspace{1cm} (3)

where $t$ is the time, $\rho$ is the density and $u$ is the velocity vector. The subscripts $g$ and $s$ represent the fluid and solid phases, respectively. Similarly, the momentum equations become

$$\frac{\partial (\alpha_g \rho_g u_g)}{\partial t} + \nabla \cdot (\alpha_g \rho_g u_g u_g) = \nabla \cdot (\alpha_g \tau_g) - \alpha_g \nabla p + \alpha_g \rho_g g + K_{gs} (u_s - u_g)$$ \hspace{1cm} (4)

$$\frac{\partial (\alpha_s \rho_s u_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s u_s u_s) = \nabla \cdot (\alpha_s \tau_s) - \alpha_s \nabla p - \nabla p_s + \alpha_s \rho_s g + K_{gs} (u_g - u_s)$$ \hspace{1cm} (5)

where $g$ is the gravitational acceleration vector, $p$ is the shared pressure, $p_s$ is the particle pressure and $K_{sg}$ is the interphase drag coefficient. Both phases are treated as Newtonian fluids. The resulting stress tensors are given by

$$\tau_g = \mu_g \left[ \nabla u_g + (\nabla u_g)^T \right] - \frac{2}{3} \mu_g (\nabla \cdot u_g) I$$ \hspace{1cm} (6)

$$\tau_s = \mu_s \left[ \nabla u_s + (\nabla u_s)^T \right] - \left( \lambda_s - \frac{2}{3} \mu_s \right) (\nabla \cdot u_s) I$$ \hspace{1cm} (7)

where $\mu$ is the dynamic viscosity, $\lambda_s$ is the solid bulk viscosity, $\tau$ is the stress tensor and $I$ is the identity tensor.
2.2 Closure modeling

A multitude of different models have been proposed to handle the various unclosed terms in these equations. For more information, the reader is referred to van Wachem et al. [26], who provides a comprehensive summary of many conventional models. Verma et al. [13] provides a study on the impact of several closure model parameters in three-dimensional cylindrical fluidized bed analyses. The models used in this work are detailed in the following sections.

2.2.1 Drag model

The interphase drag term

$$K_{gs}(u_g - u_s)$$

is a function of the interphase drag coefficient $K_{gs}$. Several drag models have been suggested. In this work the model proposed by Gidaspow [3] is used. It applies the Ergun [27] model for packed regions (where $\alpha_s > 0.2$) and the Wen-Yu [28] model for dilute regions (where $\alpha_s < 0.2$). The resulting drag coefficient, which combines form drag (caused by the particle size and shape) and skin drag (caused by friction between the fluid and a particle surface) is given by

$$K_{gs} = \begin{cases} \frac{3}{4} C_d \rho_g \alpha_s |u_g - u_s| \alpha_g^{-2.65} & \alpha_s < 0.2 \\ 150 \frac{\mu_s \alpha_s^2}{\alpha_s \rho_g d_p} + 1.75 \frac{\rho_g \alpha_s}{\alpha_s \rho_g d_p} |u_g - u_s| & \alpha_s > 0.2 \end{cases}$$

where $d_p$ is the particle diameter. The drag coefficient $C_d$, as suggested by Rowe [29], is given by

$$C_d = \begin{cases} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) & Re_p < 1000 \\ 0.44 & Re_p \geq 1000 \end{cases}$$

where the particle Reynolds number $Re_p$, as suggested by Gidaspow [3], is defined by

$$Re_p = \frac{\rho_g d_p |u_g - u_s|}{\mu_g}$$

2.2.2 Granular temperature

A model is needed to address the solid stress tensor $\tau_s$. For this, the kinetic theory of granular flow (KGTF) is applied [30,31]. From KGTF the concept of granular temperature $\Theta$, or the energy of random particle motions within the solid phase, is
introduced. This quantity must also be conserved, leading to a transport equation given by

$$\frac{3}{2} \frac{\partial}{\partial t} (\alpha_s \rho_s \Theta) + \nabla \cdot (\alpha_s \rho_s \mathbf{u}_s \Theta) = (-p_s I + \tau_s) : \mathbf{V} \mathbf{u}_s + \nabla \cdot (\kappa_s \nabla \Theta) - \gamma_s + J_{\text{vis}} + J_{\text{slip}} \tag{11}$$

where $\kappa_s$ is the conductivity of the granular energy, $\gamma_s$ is the dissipation due to interparticle collisions, $J_{\text{vis}}$ is dissipation due to viscosity, and $J_{\text{slip}}$ is the production due to turbulence.

Models are provided for these terms as follows:

$$\kappa_s = \frac{2}{g_0 (1 + e_s)} \left[ 1 + \frac{6}{5} (1 + e_s) \alpha_s g_0 \right] \left( \kappa_s, \text{dilute} \right) + 2 \alpha_s^2 \rho_s d_p g_0 (1 + e_s) \frac{\theta}{\pi} \tag{12}$$

$$\kappa_s, \text{dilute} = \frac{7.5}{384} \sqrt{\pi} \rho_s d_p \tag{13}$$

$$\gamma_s = 3 (1 - e_s^2) \alpha_s^2 \rho_s g_0 \Theta \left( \frac{4}{d_p} \sqrt{\frac{\theta}{\pi}} \mathbf{V} \cdot \mathbf{u}_s \right) \tag{14}$$

$$J_{\text{vis}} = 3 K_{gs} \Theta \tag{15}$$

$$J_{\text{slip}} = \frac{\rho_s d_p}{4 \sqrt{\pi} \Theta} \left( \frac{18 \mu_p}{d_p^2 \rho_s} \right)^2 \left| \mathbf{u}_g - \mathbf{u}_s \right|^2 \tag{16}$$

Here, $g_0$ is the radial distribution and $e_s$ is the particle-particle restitution coefficient.

### 2.2.3 Solid viscosity model

The solid viscosity $\mu_s$ has collisional, kinetic and frictional components such that

$$\mu_s = \mu_{s, \text{col}} + \mu_{s, \text{kin}} + \mu_{s, \text{fric}} \tag{17}$$

The collisional and kinetic components of the solid viscosity are modelled as

$$\mu_{s, \text{col}} = \frac{4}{5} \alpha_s^2 \rho_s d_p g_0 (1 + e_s) \frac{\theta}{\pi} \tag{18}$$

$$\mu_{s, \text{kin}} = \frac{2 \mu_{s, \text{dilute}}}{g_0 (1 + e_s)} \left[ 1 + \frac{4}{5} (1 + e_s) \alpha_s g_0 \right]^2 \tag{19}$$

$$\mu_{s, \text{dilute}} = \frac{5 \sqrt{\pi} \Theta}{96} \rho_s d_p \tag{20}$$

The bulk viscosity is calculated as

$$\lambda_s = \frac{4}{3} \alpha_s^2 \rho_s d_p g_0 (1 + e_s) \frac{\theta}{\pi} \tag{21}$$

### 2.2.4 Radial distribution model

Several models are available for the radial distribution $g_0$. In this work the model provided by Carnahan-Starling [32] is used.
\[ g_0 = \frac{1}{1 - \alpha_s} + \frac{3\alpha_s}{2(1 - \alpha_s)^2} + \frac{\alpha_s^2}{2(1 - \alpha_s)^3} \]  

(22)

2.2.5 Solid pressure model

The solid pressure term as given by Lun et al. [33] is

\[ p_s = \rho_s \alpha_s \Theta + 2\alpha_s^2 g_0 \Theta (1 + e_s) \]  

(23)

2.2.6 Frictional stress model

At high solid volume fractions, particles are in extended contact with each other. Collisions cannot be considered inelastic over a critical solid volume fraction \( \alpha_{s,f,min} \). Over this threshold, frictional components are added to the kinetic solid pressure and solid viscosity terms previously defined such that

\[ p_s = p_{s,kin} + p_{s,f} \]  

(24)

\[ \mu_s = \mu_{s,kin} + \mu_{s,f} \]  

(25)

Models offered by Johnson and Jackson [34,35] and Schaeffer [36] are often used. Srivastava and Sundaresan [37] take the added frictional pressure component \( p_{s,f} \) from Johnson and Jackson and the frictional viscosity component \( \mu_{s,f} \) from Schaeffer, combined a granular temperature term as given by Savage [38]. The resulting components are given by

\[ p_{s,f} = Fr \left( \frac{\alpha_s - \alpha_{s,min}}{\alpha_{s,max} - \alpha_s} \right)^n \]  

(26)

\[ \mu_{s,f} = p_{s,f} \frac{\sqrt{2\sin \varphi_f}}{2 \sqrt{S \cdot S + \frac{\Theta}{S}} \cdot p} \]  

(27)

\[ S = \frac{1}{2} [\nabla \bar{u}_s + (\nabla \bar{u}_s)^T] - \frac{1}{3} (\nabla \cdot \bar{u}_s) \]  

(28)

where \( \varphi_f \) is the angle of internal friction and \( \bar{u}_s \) denotes the average of the particle velocity vector. Johnson and Jackson [34], [35] proposed values for \( Fr, n \) and \( p \). In this work, the following values are used:

\[ Fr = 0.05 \]

\[ n = 2 \]

\[ p = 5 \]
2.2.7 Wall boundary condition

The no-slip boundary condition is applied to the fluid phase at the wall. For the particle phase, the boundary condition proposed by Johnson and Jackson [34] is applied. This approach accounts for partial slip velocity for the particle phase at the wall. The particle stress at the wall $\tau_{sw}$ is given by

$$\tau_{sw} = -\frac{\pi}{6} \frac{a_s}{a_{s,max}} \phi \rho_s g_0 \sqrt{3\theta} u_{s,w}$$

(29)

where $\phi$ is the specularity coefficient and $u_{s,w}$ is the particle velocity at the wall. The granular energy flux at the wall is given by

$$q_{o,w} = \frac{\pi}{6} \frac{a_s}{a_{s,max}} \phi \rho_s g_0 \sqrt{3\theta} |u_{s,w}|^2 - \frac{\pi}{6} \frac{a_s}{a_{s,max}} (1 - e_{s,w}^2) \rho_s g_0 \sqrt{3\theta}$$

(30)

where $e_{s,w}$ is the particle-wall restitution coefficient.

3 Experimental Setup

Experimental data is obtained from Makkawi et al. [21], who used electrical capacitance tomography (ECT) to obtain experimental solid volume fraction data from a cylindrical fluidized bed 13.8 cm in diameter. Glass beads with particle diameters of 350 μm and 125 μm - classified as Geldart B and Geldart A/B respectively [39] - were tested. The static bed height used was 20 cm. Ambient air was used for fluidization. Velocities of 0.26 m/s, 0.54 m/s (bubbling regime) and 0.80 m/s (slugging regime) were examined. Data was averaged between heights of 14.3 and 18.1 cm. This work examines only the bubbling regime of the Geldart B particles.

4 Numerical Setup

4.1 Simulation parameters

Table 1 contains the simulation parameters applied to this study. The solid volume fraction is time-averaged between 5 seconds and 40 seconds. Table 2 summarizes the closure models used.
In OpenFOAM, the Srivastava-Sundaresan frictional stress model is not currently available as part of the release. As the model combines approaches of both Johnson-Jackson and Schaeffer, which are both available in OpenFOAM, their implementations in OpenFOAM are used to build the Srivastava-Sundaresan model. Once the model is coded in C++ and properly structured within the `twoPhaseEulerFoam` directory, the solver is re-compiled to include the new frictional stress model.

### 4.2 Boundary and initial conditions

#### 4.2.1 Fluid volume fraction

Initially, the air volume fraction is set as 0.40 within the static bed region, or $0 \leq y \leq 0.20$ m. Above the static bed where no particles are present, the volume fraction is set to 1. To accomplish this in OpenFOAM, it is convenient to set the initial fluid volume fraction to a uniform value of zero everywhere and use the `setFields` utility provided by OpenFOAM to set the volume fractions of all grid points within a specified area to a specified value. In this case, a default value of 1 is applied to the entire cylindrical volume. Then a value of 0.40 is applied to the cylindrical region $0 \leq y \leq 0.20$.

At the inlet, outlet and wall boundaries, the volume fraction boundary condition is set to zero gradient.

### Table 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simulation time</td>
<td>40 s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>0.138 m</td>
</tr>
<tr>
<td>Riser height</td>
<td>0.6 m</td>
</tr>
<tr>
<td>Initial bed height</td>
<td>0.2 m</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>350 µm</td>
</tr>
<tr>
<td>Particle density</td>
<td>2500 kg/m³</td>
</tr>
<tr>
<td>Maximum packing</td>
<td>60%</td>
</tr>
<tr>
<td>Particle-particle restitution coefficient</td>
<td>0.8</td>
</tr>
<tr>
<td>Particle-wall restitution coefficient</td>
<td>0.9</td>
</tr>
<tr>
<td>Specularity coefficient</td>
<td>0.6</td>
</tr>
<tr>
<td>Angle of internal friction</td>
<td>28.5°</td>
</tr>
<tr>
<td>Air density</td>
<td>1.225 kg/m³</td>
</tr>
<tr>
<td>Air viscosity</td>
<td>$1.77 \times 10^{-5}$ m²/s</td>
</tr>
<tr>
<td>Volume fraction</td>
<td>1.0</td>
</tr>
<tr>
<td>Fluid volume fraction</td>
<td>0.40</td>
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</tbody>
</table>

### Table 2

<table>
<thead>
<tr>
<th>Table 2: Closure model summary</th>
</tr>
</thead>
<tbody>
<tr>
<td>Drag</td>
</tr>
<tr>
<td>Solid pressure</td>
</tr>
<tr>
<td>Conductivity</td>
</tr>
<tr>
<td>Bulk solid viscosity</td>
</tr>
<tr>
<td>Radial distribution</td>
</tr>
<tr>
<td>Frictional stress</td>
</tr>
<tr>
<td>Solid viscosity</td>
</tr>
<tr>
<td>Wall boundary condition</td>
</tr>
</tbody>
</table>
4.2.2 Solid volume fraction

Using the same procedure specified for the fluid volume fraction, the solid volume fraction is set to 0.6 within the bed region and 0 elsewhere. The same boundary conditions apply.

4.2.3 Pressure

The pressure throughout the cylindrical volume is set to an ambient condition of 101325 Pa. At the outlet, the pressure remains at ambient condition. At the inlet and walls, a \textit{fixedFluxPressure} boundary condition is applied. In OpenFOAM, the pressure gradient is calculated such that the velocity boundary condition specifies the boundary flux.

4.2.4 Temperature

As the case in this study is not examining heat transfer, both the air and solid temperatures are initially set to 297 K throughout the region. Inlet and outlet air boundary conditions are also set to 297 K. At the walls, a zero gradient boundary condition is applied to the fluid phase. Zero gradient conditions are applied to inlet, outlet and wall boundaries for the solid phase.

4.2.5 Granular temperature

The granular temperature is initialized to zero. At the inlet, a fixed value of zero is applied. At the outlet, a zero gradient condition is applied. The Johnson-Jackson boundary condition is applied at the wall boundary.

4.2.6 Fluid velocity

The fluid velocity field is initialized to 0.54 m/s. At the inlet, an \textit{interstitialInletVelocity} boundary condition is applied. In OpenFOAM, this calculates the local interstitial velocity as the specified inlet velocity divided by the local fluid volume fraction. In this case, the specified inlet velocity is 0.54 m/s. The volume fraction is a calculated field. At the outlet, a \textit{pressureInletOutletVelocity} condition is applied. In OpenFOAM, this boundary condition is used at boundaries where pressure is specified. It applies a zero gradient condition to any outflow at the boundary and calculates the velocity for any inflow at the boundary. At the wall boundary, the no-slip condition results in a fixed value of zero velocity.
4.2.7 Solid velocity

The solid phase velocity is initialized to zero. At the inlet and outlet, fixed value conditions of zero are applied. At the wall, the Johnson-Jackson boundary condition is applied, resulting in a partial-slip condition.

4.3 Domain discretization

The flow configuration consists of a cylinder whose cross section is discretized using four grid construction methods: cut cell, curved Cartesian, cylindrical and hybrid. The cut cell begins with a structured Cartesian grid and uses trimmed cells around the specified boundary to conform to the cylindrical shape. All cells outside of the boundary are removed. To accomplish this in OpenFOAM, the cylindrical geometry is created in a .stl file and included in the case directory. A complex meshing utility named snappyHexMesh, which is included with OpenFOAM, fits the Cartesian grid to the boundary. The resulting grid loses some resolution of the wall boundary and creates a more complex mesh at the wall, but retains a structured Cartesian grid away from the wall curvature. A cut cell mesh is shown in Figure 1.

In the curved Cartesian grid, a structured Cartesian mesh is specified and is fit to the cylindrical wall using a four-corner approach. In this way, the curvature of the wall is preserved. However, very small cells are created at some points near the wall. A curved Cartesian mesh is shown in Figure 2.

The cylindrical mesh is well-suited to handle the cylindrical geometry studied in this work as it maintains the wall curvature. A cylindrical mesh is shown in Figure 3.

A hybrid mesh is also examined using a five-block o-grid type topology. It applies a structured mesh in the center of the domain and blends into a cylindrical mesh around the wall. A hybrid mesh is shown in Figure 4.
4.4 Approach

To compare the grid geometries, a mesh independent solution is sought for each construction method. The accuracy of the different mesh arrangements are discussed individually. The mesh independent resolutions for each arrangement are then re-run using 24 Intel Xeon CPU E5-2680 2.8GHz processors. Computing resources were available through the Northeastern University high performance computing Discovery Cluster. Results are presented in the following section.
5 Results

5.1 Fluidized bed behavior

The fluid volume fraction, often referred to as the void fraction, is used to study the gas-solid flow dynamics within fluidized beds. Instantaneous void fraction profiles for the curved Cartesian, cut cell and cylindrical grids are shown in Figure 5. Slices are taken at $\theta = 0^\circ$. Three-dimensional contours of the void fractions are shown in Figure 6. Here, contours of $\alpha_g = 0.7$ are shown. As the small bubbles rise through the height of the bed, they interact and coalesce, forming larger voids.

Figure 7 shows time averaged void fractions. Again, slices are taken at $\theta = 0^\circ$. As previously mentioned, the solid volume fraction is time averaged from 5 seconds to 40 seconds. The results are typical for bubbling fluidized beds. The effect of near-wall interactions are clearly visible in Figure 7. The partial-slippage of the particle phase results in particles collecting more along the cylindrical wall. As they rise and coalesce, bubbles are forced toward the centerline of the bed. In Figure 8, void fraction cross sections at a height of 16.2 cm are shown. From these profiles, it is seen that although there are variations in the instantaneous bubble dynamics predicted via different meshes, the mean fields shown in Figure 7 are almost insensitive to the choice of mesh configuration. However, the mean void fraction exhibits considerable variation in azimuthal direction, as illustrated in Figure 8.

5.2 Post-processing

To account for the azimuthal variation, values are averaged azimuthally between $0^\circ$ and $180^\circ$ (represented as positive radial values) and $180^\circ$ to $360^\circ$ (represented as negative radial values). As Makkawi et al. [21] discussed, the values are also averaged within bed heights of 14.3 cm and 18.1 cm.
Figure 5: Instantaneous void fraction
Figure 6: Three-dimensional isosurfaces of void fraction ($\alpha_g = 0.7$)
Figure 7: Time-averaged void fraction
5.3 Resolution studies

5.3.1 Curved Cartesian

Figure 9 shows the grid resolution study for the curved Cartesian mesh method. In general, the predictions from OpenFOAM compare favorably with the experimental data. As the mesh is refined, the centerline void fraction decreases and the solution deviates from the experimental data. However this behavior is consistent with the Cartesian cut cell results from MFIX. Based on the results the 27x27 grid is chosen for further analysis.

5.3.2 Cut cell

Figure 10 shows the grid resolution study for the curved Cartesian mesh method. Similar to the curved Cartesian method, the cut cell method also under-predicts the centerline void fraction. Again, the OpenFOAM results show good comparison with
experimental data and are consistent with the cut cell results from MFiX. For performance testing, the 31x31 cut cell grid is chosen.

Figure 9: Curved Cartesian grid resolution

Figure 10: Cut cell grid resolution
5.3.3 Cylindrical

For the cylindrical mesh, both radial and azimuthal studies were performed. Figures 11 and 12 show the impact of the radial and azimuthal grid resolutions respectively. The cylindrical grids show predictions closer to the experimental data than those of the cut cell and curved Cartesian shown in previous sections. The azimuthal resolution does not have a significant impact on the results. The radial resolution however has significant impact, primarily in the center region of the bed. A grid resolution of 18 radial and 40 azimuthal cells is used for performance evaluation.

5.3.4 Hybrid

For the hybrid o-grid type mesh, the azimuthal and radial results from the cylindrical mesh study are used. Using the azimuthal resolution from the cylindrical study, a center section grid spacing of 13 azimuthal cells per quadrant is used, resulting in a 13x13 center section. This also dictates that 13 azimuthal cells per quadrant be used, resulting in 52 azimuthal cells. Using the radial spacing from the cylindrical study results in 10 cells radially in the outer section. The results for this mesh are provided in the following section.

Figure 11: Cylindrical mesh - radial grid resolution
5.4 Mesh geometry efficiency

Table 3 summarizes the meshes chosen to evaluate performance. These cases were then run on 24 processors each using the same computing cluster. Before discussing the efficiency, the resulting predictions of bed characteristics are discussed.

<table>
<thead>
<tr>
<th>Mesh Type</th>
<th>Grid Size</th>
<th>Cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curved Cartesian</td>
<td>27x27</td>
<td>87,480</td>
</tr>
<tr>
<td>Cut Cell</td>
<td>31x31</td>
<td>89,880</td>
</tr>
<tr>
<td>Cylindrical</td>
<td>r=18, θ=40</td>
<td>86,400</td>
</tr>
<tr>
<td>Hybrid (o-grid type)</td>
<td>13x13, r=10, θ=52</td>
<td>82,680</td>
</tr>
</tbody>
</table>

The void fraction profiles are shown in Figure 13. The solutions provided by each mesh arrangement are very similar. The cut cell has the most deviation from the experimental results at the centerline, but still shows reasonably good agreement.
To examine the void fraction from a slightly different perspective, the time-averaged void fraction along the height of the cylinder at the centerline is shown in Figure 14. This provides a sense of the bed height predicted by the simulations. The profile exhibited by all the mesh arrangements is characteristic of a bubbling fluidized bed. Though some variation is seen in the bed region (where the solid phase is present), all the mesh arrangements show good agreement in the predicted height of the bed.

The pressure drop across the cylinder height is given in Figure 15. As with the void fraction, the values are taken from the cylinder center. The predictions show negligible difference. As with the void fraction, the cut cell configuration deviates the most, but still shows reasonable agreement with the other meshes.
The time-averaged solid phase velocity magnitude is shown in Figure 16. Slices are taken at $\theta = 0^\circ$ and the plot is isolated to the bed region. The color contour depicts velocity magnitude and vectors show direction. As with void fraction and pressure, the results are similar across the mesh arrangements.
Figure 16: Time-averaged solid phase velocity magnitude
Figures 13 through 16 serve to show that, for grid independent solutions, the analyzed mesh construction methods predict very similar behavior in terms of time-averaged void fraction, pressure drop and solid velocity. The fact that the grid independent solutions produce similar results shows consistency in the OpenFOAM analysis. In the resolution studies, it was shown that the mesh has a significant impact on accuracy and performance of the solution. As a mesh independent solution is sought, the predictions become independent of the grid construction method. However, the important issue is that the rate of convergence to grid independent solution, and thus computation time, are different for various meshing strategies. In addition, the grid sizes of the mesh independent solutions vary greatly. To evaluate the computational performance of each mesh arrangement, the mesh independent solutions were recalculated using the computational resources discussed in Section 4.4. Table 4 provides the run times for the mesh independent cases. Given the decrease in cells in the hybrid mesh, it is logical that it would have the fastest runtime. In terms of computational service units, the difference in runtimes has a significant impact on the cost of a fluidized bed simulation.

<table>
<thead>
<tr>
<th>Table 4: Computational performance results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Curved Cartesian</td>
</tr>
<tr>
<td>Cut Cell</td>
</tr>
<tr>
<td>Cylindrical</td>
</tr>
<tr>
<td>Hybrid (o-grid type)</td>
</tr>
</tbody>
</table>

6 Conclusion

This study concentrates on three-dimensional fluidized bed simulations and how they are affected by the computational grid chosen to model the system. The Eulerian-Eulerian formulation, discussed in the Section 2, is employed to describe the gas-solid flow in fluidized beds. Simulations are carried out in OpenFOAM. To evaluate the accuracy of the predictions, void fraction profiles are analyzed. Resolution studies are performed for curved Cartesian, cut cell and cylindrical meshes. For the cylindrical mesh, both radial and azimuthal resolutions are considered.
Using grid independent solutions found in the resolution studies, the computational performance of the grid configurations are compared against each other. It is shown that significant savings in terms of computational cost can be realized by choosing an efficient mesh arrangement. In the case of this work, for a cylindrical fluidized bed, a hybrid o-grid type mesh produces results similar to those obtained by other meshes, but with a much faster runtime.

A future extension of this work is to conduct simulation of two-phase reacting flow in fluidized beds. Such extension is useful to study coal and biomass combustion and gasification. Due to the computational cost of such simulations, it is essential to investigate the impact of domain decomposition method on parallel computational efficiency for various mesh configurations.
References


