MODELING AND SIMULATION OF POLYDISPERSED MULTIPHASE FLOW

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1 Introduction

Polydispersed multiphase flows are present in several natural and industrial processes, and involve a series of physical phenomena, such as: transfer of mass, momentum and energy. In bubble column chemical that are used in the biochemical and petrochemical industries, reactor efficiency significantly depends on interfacial area of the bubbles and the resident time. Therefore, the particle size distribution (PSD) is a parameter whose behavior is important to control this process. In material science, the precipitation reaction is another good example of polydispersed multiphase flow. In this case, reaction happens in a liquid phase with some chemical substances that react to form a solid with some specific features. The final market value of the crystallized product is strongly dependent on its PSD. For these reasons, modeling and simulation of polydispersed multiphase flow is critically important. In this work, we describe a computational framework to simulate polydispersed multiphase flows based on population balance equations (PBE), and we also discuss which numerical methods is suitable to couple the solution of PBE with CFD simulations.

2 Mathematical Model

Three main approaches can be used to model polydispersed multiphase flows: the fully-resolved, the Lagrangian point-particle and the Eulerian-Eulerian model [6]. In the Eulerian-Eulerian (E-E) models, the phase equations are derived for their mean variables, that are closed by constitutive relations obtained from empirical data [3]. This average procedure yields equations with a reasonable computational cost and accuracy for complex problem in large scale. Nonetheless, this model by itself can not capture particle-particle interactions, such as aggregation and breakage phenomena. In order to overcome this limitation a mesoscale framework called population balance model (PBM), which is the conservation equation for the number of particles represented by a number density function (NDF) [6], can be combined with a multi-fluid flow formulation [5] to predict the particle-particle and particle-fluid interactions.

2.1 Eulerian Multiphase Model

The Eulerian-Eulerian multiphase equations are derived by the averaging process in conservation equations. The result of this averaging procedure yields the mass conservation equation for the each phase below [6]:

$$\frac{\partial(r_\alpha\rho_\alpha)}{\partial t} + \nabla.(r_\alpha\rho_\alpha\mathbf{u}_\alpha) = \Gamma_\alpha, \tag{1}$$

where ρ_α is the density, Γ_α is a mass source term and $\mathbf{u}_\alpha$ is the velocity of the phase α, where $\alpha = 0 \cdots N$. In this equation, the volume fraction, r_α, appears as the probability of a phase α exists in the space and time regarding all possible realizations.

Extending the same procedure to momentum conservation equations for the α phase, the following averaged equation is obtained:

$$\frac{\partial(r_\alpha\rho_\alpha\mathbf{u}_\alpha)}{\partial t} + \nabla.(r_\alpha\rho_\alpha\mathbf{u}_\alpha\mathbf{u}_\alpha) = -r_\alpha\nabla p_\alpha + \nabla.(r_\alpha\rho_\alpha\tau_\alpha^{\mathbf{eff}}) + r_\alpha\rho_\alpha\mathbf{g} + \Gamma_\alpha\mathbf{u}_\alpha + \sum_{\substack{\beta=0\\\beta\neq\alpha}}^{\beta=N}\mathbf{M}_{\alpha,\beta}, \tag{2}$$

where $\tau_\alpha^{\mathbf{eff}}$ is the effective stress tensor, which has the effects of viscous stress tensor and turbulent stress tensor. $\mathbf{M}_{\alpha,\beta}$ represents the interfacial momentum exchanged between the phases α and β. It is usually broken into drag force, lift force, virtual mass force, average interfacial pressure and shear stress at the interface.

2.2 Population Balance Modeling

The PB-CFD coupling has proved to be well-suited to predict polydispersed multiphase flows [5, 1, 2]. In this work, the following inhomogeneous monovariate PBE with an additive internal variable, x, is used:

$$\frac{\partial f(x,\mathbf{z},t)}{\partial t} + \nabla_z.[\mathbf{u_d}f(x,\mathbf{z},t)] = S(x,\mathbf{z},t) + R(x,\mathbf{z},t), \tag{3}$$

where $S(x,\mathbf{z},t)$ is an additional source term, x is an internal variable for diameter, $\mathbf{z}$ is the physical space coordinates and $R(x,\mathbf{z},t)$ is given by the equation below:

$$R(x, \mathbf{z}, t) = \mathcal{L}_b f(x, \mathbf{z}, t) + \mathcal{L}_a f(x, \mathbf{z}, t). \quad (4)$$

The $\mathcal{L}_b$ and $\mathcal{L}_a$ are, respectively, the breakage and aggregation operators.

3 PB-CFD coupling with DQBMMs

The DQBMM-PB-CFD coupling is very similar to QBMM-PB-CFD coupling [5]. Again, each Gauss-Christoffel quadrature node is assigned to one dispersed phase α, and when their abscissas are the particle volume, the weighted abscissa, ζ_α, is equivalent to its volume fraction in an incompressible flow. Furthermore, if the particles are considered spherical, the particle volume can be converted into the particle diameter, and therefore, used to calculate the interfacial force between the continuous and dispersed phases in each CFD cell.

4 Results and Discussions

In order to verify the PB-CFD coupling with DQBMMs, we applied this approach with some tool models. The DQBMM-PB-CFD code verification is carried out in a two dimesional Backward Facing Step (BFS) geometry, due to its simplicity and well-defined recirculation zones, where the effects of particle interaction are predominant. DQBMM-PB-CFD code, implemented in OpenFOAM, is simulated with unrealistics problems with breakage and aggregation kernels describe in the following.

4.1 Simultaneous breakage and aggregation cases

The simultaneous breakage and aggregation problem proposed by McCoy and Madras [4] is simulated to compare the results of DQMoM, DuQMoGeM and Direct DuQMoGeM using 4 moments. Regarding to the simulations result, from Figure 1, one can see that, the recirculation zones on the BFS is evident right after the step. In these regions the residence time of dispersed phase is longer and the aggregation and breakage effects are higher.

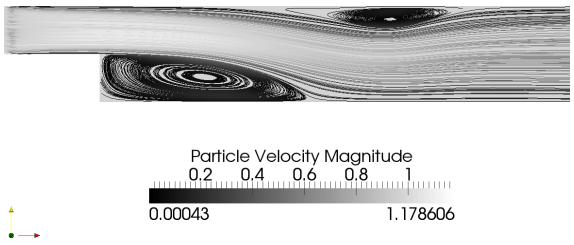

Figure 1: Velocity magnitude of the dispersed phase for breakage case with 6000 nodes mesh and tolerance of 1×10^{-6} at 0.3 seconds.

From Figure 2, we can observe that in recirculation zone the emulsion starts to break as was expected. This result was represented by Silva and Lage [5] using tradicional DQMoM.

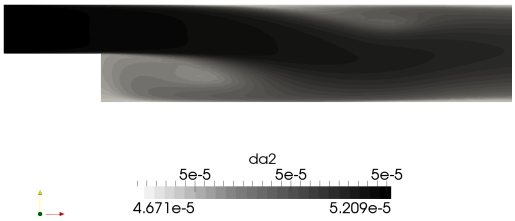

Figure 2: Diameter of dispersed phase with 6000 nodes mesh and tolerance of 1×10^{-6} at 0.3 seconds.

5 Conclusions

In this work, a polydispersed multiphase flow model using dual quadrature-based moments methods were implemented in OpenFOAM and parallelized on GPUs. In order to verify the code, the DQBMM-PB-CFD coupling were applied to an oil-water emulsion and their results were compared to the same code using DQMoM. The results were similar. However, we can consider that the dual quadrature-based moments methods are more acurate, once they can control the quadrature error present in DQMoM.

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