

Approach to a hybrid Eulerian-Eulerian-Lagrangian Model for Gas-Solid Simulations

Daniel Hirche^{1,2*}, Fabian Birkholz^{1,2}, Olaf Hinrichsen^{1,2}

1 Technical University of Munich, Department of Chemistry, Lichtenbergstraße 4, 85748 Garching, Germany

2 Technical University of Munich, Catalysis Research Center, Ernst-Otto-Fischer-Straße 1, 85748 Garching, Germany

**Corresponding author: daniel.hirche@ch.tum.de*

Highlights

- Development of a fully coupled two fluid model with a discrete element model
- Combining the speed of two fluid model and the accuracy of the discrete element model
- Adjustable ratio of Euler-solid and Lagrangian particles for optimal speed/accuracy

1. Introduction

Computational Fluid Dynamics (CFD) simulations for modelling two-phase, gas-liquid, gas-solid or liquid-solid flows, has become more applicable in industry than ever due to increasing computational performance. The simulations are based on either a two fluid model (TFM) or an Eulerian-Lagrangian (EL) model. The TFM simulates for each component a continuum, while for the EL-model the fluid is still handled as a continuum, but the disperse component is simulated with a discrete element method (DEM). It is obvious that the TFM has its advantages in simulation speed, but inaccuracies in terms of results, and the EL-model model results are very accurate, but simulation speed is the main disadvantage. Therefore, a coupled solver is developed, combining the TFM and Lagrangian model and validated on a fluidized bed benchmark.

2. Methods

The TFM is based for a fluid (f) and a solid phase (s) on the continuity (1) and momentum equations for the fluid (2) and the solid phase (3) coupled with a moment exchange coefficient β .

$$\frac{\partial(\alpha_i \rho_i)}{\partial t} + \nabla \cdot (\alpha_i \rho_i \mathbf{U}_i) = 0 \quad (1)$$

$$\frac{\partial(\alpha_f \rho_f \mathbf{U}_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \mathbf{U}_f \mathbf{U}_f) = -\alpha_f \nabla p + \alpha_f \rho_f \mathbf{g} + \nabla \cdot (\alpha_f \underline{\underline{\tau}}_f) + \beta(\mathbf{U}_s - \mathbf{U}_f) \quad (2)$$

$$\frac{\partial(\alpha_s \rho_s \mathbf{U}_s)}{\partial t} + \nabla \cdot (\alpha_s \rho_s \mathbf{U}_s \mathbf{U}_s) = -\alpha_s \nabla p - \nabla p_s + \alpha_s \rho_s \mathbf{g} + \nabla \cdot (\alpha_s \underline{\underline{\tau}}_s) + \beta(\mathbf{U}_f - \mathbf{U}_s) \quad (3)$$

The DEM is based on particle tracking and the momentum equation (4) for particles is solved according to Newton's second law for every single particle.

$$m_{p,i} \frac{d\mathbf{v}_{p,i}}{dt} = m_{p,i} \frac{d^2 \mathbf{x}_{p,i}}{dt^2} = -V_{p,i} \nabla \cdot p + \frac{V_{p,i} \beta}{\alpha_{p,i}} (\mathbf{U}_f - \mathbf{v}_{p,i}) + m_{p,i} \mathbf{g} \quad (4)$$

The newly developed Eulerian-Eulerian-Lagrangian (EEL) solver simulates the fluid phase in an Eulerian framework. The solid phase is divided in an Eulerian and Lagrangian framework. The ratio of how many particles are simulated in an Eulerian and Lagrangian framework is variable. In order to model particle interactions, e.g. collisions, between DEM-particles and Eulerian particles, every Eulerian particle is transformed to a DEM-particle in the framework. The number of particles is dependent on the phase fraction of the solid phase α_s , the volume of the cell V_c and the volume of a single particle $V_{p,i}$. Figure 1A and 1B illustrate the transformation of certain phase fraction of particles to DEM-particles. The coupling between the DEM-particles and Euler-fluid was achieved by adding an additional source term $\beta_p (\bar{\mathbf{v}}_p - \mathbf{U}_f)$ to equation (1), while β_p is the momentum exchange coefficient for DEM-particles and $\bar{\mathbf{v}}_p$ is the mean velocity of DEM-particles based on the respective mesh cell. The coupling between DEM-particles and Euler-particles is realized by transforming the Euler-particles to inactive DEM-particles. Collisions between active and inactive DEM-particles are detected and accounted for. The proposed algorithm was implemented in the opensource code OpenFOAM[®] [1] version 4.1.

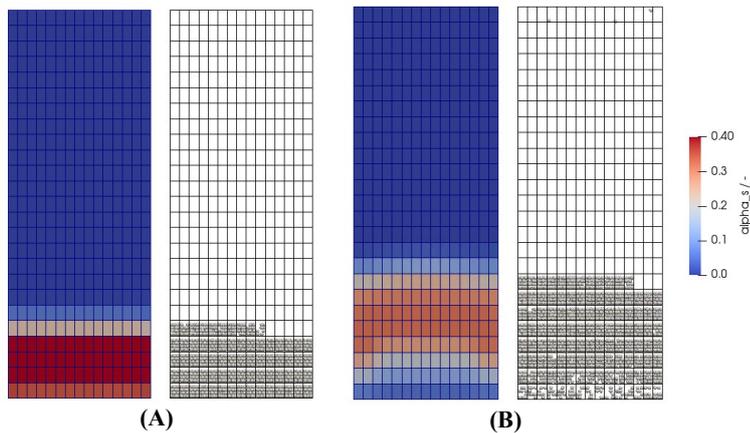


Figure 1. Volume Fraction of particles for Eulerian phase (left) and transformation to inactive DEM-particles (right) at initial state (A) and after 1 s (B).

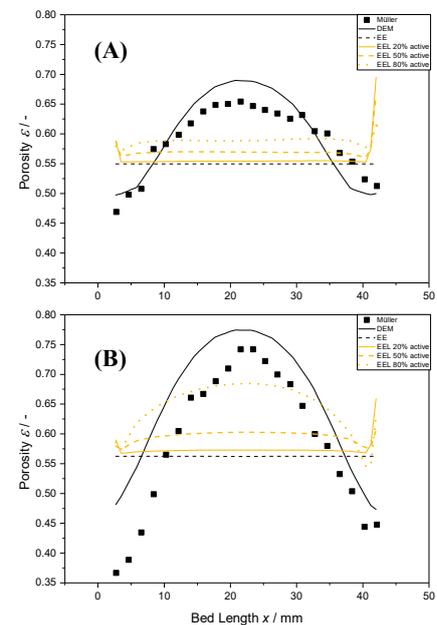


Figure 2. Simulation results obtained with different solvers compared with MR measurements by Müller et al. [2] at reactor height of 16.8 mm (A) and 31.2 mm (B).

3. Results and discussion

As a validation, the experimental data from a fluidized bed of poppy seeds in air by Müller et al. [2] obtained by MR measurements will be compared with the results of a Euler-DEM-solver (*DPMFoam*), a TFM-solver (*twoPhaseEulerFoam*) and the new EEL-solver with different ratios of Eulerian- and DEM-particles (20 %, 50 % and 80% active DEM-particles). Figure 2A and 2B show the simulation results and experimental data for porosities at different heights of the reactor ϵ . The results of the Euler-DEM-solver predict the porosity very well but tend to over-predict at greater heights of the bed. The results of the TFM-solver are not satisfactory for both heights, as it shows a uniform distribution of the porosity across the bed. The results of the new EEL-solver with different ratios of DEM to Eulerian-particles show better results than the TFM-solver. More DEM-particles than Eulerian-particles for the EEL-solver give overall more accurate results, but the results are not satisfactory due to an inhomogeneous distribution of Eulerian and active DEM-particles

4. Conclusions

A fully coupled hybrid solver with TFM and DEM was developed. The fluid phase is treated as an Eulerian-continuum, while the solid phase can be adjusted to be simulated as an Eulerian-continuum and lagrangian particles with different ratios. The results of the EEL-solver are highly dependent on the ratio of Eulerian to DEM-particles. The necessity in a homogeneous distribution between Eulerian and DEM-particles is given and will be developed. Furthermore, the solver can be modified to simulate a three-phase flow.

References

- [1] H.G. Weller, G. Tabor, H. Jasak, C. Fureby, A tensorial approach to computational continuum mechanics using object-oriented techniques, *Computers in Physics* 12 (1998) 620-631.
- [2] C.R. Müller, S. Scott, D. Holland, B. Clarke, A. Sederman, J. Dennis, L. Gladden, Validation of a discrete element model using magnetic resonance measurements, *Particuology* 7 (2009) 297-306.

Keywords

Two-Phase-Modeling; Discrete-Element-Model; Fluidized Bed; OpenFOAM®