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Application of an advanced coupled EMMS-TFM model to a pilot scale CFB carbonator

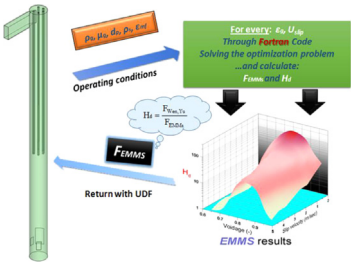
Zeneli M.*, Nikolopoulos A., Nikolopoulos N., Grammelis P., Kakaras E.

Centre for Research and Technology Hellas, Chemical Process & Energy Resources Institute (CERTH/CPERI), Athens Branch: Egialias 52, Marousi, GR-15125 Athens, Greece

HIGHLIGHTS

- CFD simulation for a pilot-scale carbonator.
- Comparison between EMMS and Gidaspow drag schemes.
- Implementation of a new model for the clusters diameter in EMMS.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper focuses on the CFD simulation of a CFB pilot-scale carbonator of a 1 MW_{th} DFB installation located at TU Darmstadt (TUD). The carbonator riser height and diameter are 8.661 m and 590 mm, respectively. The state-of-the-art TFM approach is applied while the inter-phase drag coefficient is simulated using a new configuration of the sub-grid EMMS drag model. This configuration incorporates a new approach for the determination of the clusters diameter taking into account the geometrical limitations that the riser diameter poses to the meso-scale structures. The conventional Gidaspow model and the EMMS scheme are tested simultaneously along with the grid density effect. Two mesh densities, one coarse, and one dense are applied, i.e. 31,207 and 285,369 hexahedral elements. The mean ratio of the equivalent cell size to particles diameter (D_{cell}/D_p) is 465.64 and 222.67, respectively. Except for the grid density effect on the solution results, the wall treatment boundary conditions are investigated, as far as particulates are concerned, through a parametric study on the specularity coefficient values (0.01, 0.1, 0.6 and 0.99) implemented in the partial slip model. Finally, the heterogeneous carbonation reaction is incorporated to the model and a study of the influence of the hydrodynamics on the carbon dioxide capture is investigated. Simulation results are averaged over a time period of 15 s, while the pressure measurements are compared with the corresponding experimental data. Results for pressure converge well with the experimental results for pressure measurements along the riser, when the EMMS model is applied, while it is worth mentioning that this drag model reproduced an almost grid independent solution. For the CO_2 concentration at the riser exit, the averaged for 65 s value converges well with the respective measured value.

1. Introduction

Circulating fluidized bed (CFB) is a typical technology for gas–solid reactions, that is used in a wide range of industrial applications, such as biomass gasification, pyrolysis, combustion and fluid

* Corresponding author. Tel.: +30 211 1069 507.
E-mail address: zeneli@certh.gr (M. Zeneli).

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catalytic cracking, just to name a few (Kunii, 1980). The calcium looping concept (CaL), the second most mature post-combustion capture technology following amine scrubbing (Charitos et al., 2012), utilizes such reactors for an effective CO_2 capture. First proposed by Shimizu et al. (1999) this process is performed through a dual fluidized bed facility (DFB), which comprises two reactors, named as calciner and carbonator. Inside these reactors multi-phase gas–solid heterogeneous reactions, one endothermic and one exothermic are taking place, respectively. The carbonator is the heart of this process; inside this reactor CO_2 is captured by the calcium oxide particles (CaO) forming calcium carbonate ($CaCO_3$). The calcium oxide particles are then regenerated in the calciner and transported back to the carbonator, while a lean CO_2 stream is released almost ready for storage. The unit modeled in the present work is a pilot-scale CFB carbonator part of the 1 MW_{th} DFB installation located at Darmstadt University (Ströhle et al., 2014) which is the second largest in the world (Duelli et al., 2015).

Many investigators worldwide have considered as a crucial issue the accurate and efficient simulation of CFB reactors, aiming to their up-scaling for industrial uses. In most of the cases the simulation only of the riser is preferred over the full loop (Xie et al., 2008; Zhou and Wang, 2014). This strategy is in general preferred due to its lower computational cost (Yang et al., 2003) as long as the appropriate boundary conditions for the solids inlet and the riser exit are applied (Li et al., 2014). On the other hand, only few three dimensional studies are available in the literature for a full loop simulation, and these are mainly concentrated to lab-scale units in the range of 100 kW_{th}. This is owed to the fact that even if such an approach is considered as the most accurate and valuable for an optimal fluidized bed design and operation (Chen, 2006), it is at the same time computationally very expensive. The most recent work is that of Wang et al. (2014a) who has applied the CPFD methodology in a CFB simulation with a loop seal. Previously Chu et al. (2007) conducted a 3D CFB full loop simulation using the discrete particle method (DPM). Zhang et al. (2008) applied the Eulerian two-fluid model combined with the energy-minimization multi scale scheme (EMMS) to study the hydrodynamics of a semi-industrial CFB reactor and two years later implemented their work in a 150 MW CFB boiler simulation (Zhang et al., 2010). Finally, Nikolopoulos et al. (2013), Zeneli et al. (2013) used the coupled Eulerian approach with the EMMS model for the simulation of a 3D CFB carbonator cold model.

In any case, the gas–solid flow characteristics inside a CFB are really complex and difficult to quantify. Nevertheless, owed to parallel computing availability, and rapid upgrade of CPU and GPU hardware that allow for a considerable acceleration of the calculations, the numerical methods and algorithms of computational fluid dynamics (CFD) have become a powerful tool towards achieving this target. In this context, two approaches have been proposed for the solution of the multiphase flow in a fluidized bed reactor; i.e. the Eulerian–Eulerian and (ii) the Eulerian–Lagrangian approach. The Eulerian–Eulerian two-fluid model (TFM), which is adopted in the present study, treats the gas and the solid phase as interpenetrating continua (Ding and Gidaspow, 1990; Gidaspow, 1994). This model has been extensively employed in many areas, especially in the fluidized bed simulations due to its low computational cost compared to Eulerian–Lagrangian models that explicitly model the inter-particle interactions, such as that of Discrete Elements Method (DEM) (Chen and Wang, 2014; Tsuji et al., 1992; Zeneli et al., 2014). Alternatively, MP-PIC methods (Andrews and O'Rourke, 1996; Li et al., 2012; O'Rourke and Snider, 2012), which implicitly simulate those interactions allow for a reduction of the associated CPU cost. This approach has gained popularity recently and seems promising. Some of its advantages are (Sundaresan, 2011): (a) the inclusion of particle size distribution (PSD) with a comparatively low computational cost, (b) the track of a great amount of particle parcels, and (c) the straightforward simulation of wall boundary conditions. Nonetheless, this approach has not been in depth investigated compared to the Eulerian TFM, which still remains to be the most mature methodology for the modeling of fluidized bed reactors. However, even in the case of the TFM that has been thoroughly studied, further research is required.

A parameter of crucial importance in TMF is the drag coefficient between the gas and the particulate phase. Up to present, several models that predict the inter-phase drag coefficient have been proposed in the literature. Conventional drag laws, as the ones given by Wen and Yu (1966), Gidaspow (1994) and Syamlal and O'brien (1989) over-predict the drag force induced on the solid particles by the gas phase, especially in cases where a coarse grid is used (Hartge et al., 2009; Wang et al., 2008). This is owed to the fact that the solid particles inside a fluidized bed reactor are heterogeneously dispersed, forming dynamic meso-scale structures, such as clusters, bubbles, streamers (Senior and Brereton, 1992) etc. These heterogeneous formations have a strong effect on the momentum, heat and mass transfer and the achievable conversion rates of a fluidized system (Wang et al., 2008; Zhou and Wang, 2015). For their quantification and accurate prediction either an extremely fine grid, which would increase the computational cost considerably, or a proper sub-grid model that takes into account such meso-scale structures should be used (Lu et al., 2009; Cloete et al., 2015).

The importance of sub-grid modelling has been addressed by several research groups. In Princeton group a filtered drag coefficient has been presented for Geldart A particles in a periodic domain (Igci et al., 2008). A drag correlation similar to Princeton group has been proposed by Simonin's group with the main difference that the filter length is dimensionalised with the bed diameter instead of the terminal settling particle velocity (Parmentier et al., 2012; Schneiderbauer et al., 2013). Kuiper's group presented a drag force model applicable to Geldart B and D particles in bubbling fluidized beds using coarse mesh (Wang and Liu, 2010). Finally, a sub-grid model that has been implemented the last decades in fluidized bed simulations is the energy minimization multi-scale model (EMMS).

The (EMMS) model is a sub-grid scale model that takes into account the effect of the heterogeneous formations on the determination of the momentum exchange coefficient, avoiding the application of a dense grid. This model was first introduced by Li and Kwauk (1994) for the steady flow inside a circulating fluidized bed reactor. Wang et al. (2008), Yang et al. (2003) developed an improved version of the model taking into account particle acceleration and the effective inter-phase interaction. Wang et al. (2009) proposed an EMMS model for Geldart B particles in a cold dense circulating fluidized bed. All of the abovementioned studies use as a key parameter for the EMMS model the cluster size. This is not always the case; some researchers, apply the EMMS theory by incorporating in the model the bubble size (Hong et al., 2014). This is the so called bubble-based EMMS model, which was first proposed by Shi et al. (2011). The latter model is more theoretically sound for bubbling fluidized bed reactors. For a CFB reactor though, as the one modeled in the present work, the accurate quantification of the cluster size is considered as a key parameter for an accurate EMMS model.

The precise prediction of the cluster size has been a major issue that has not yet been solved. This is owed to the fact that clusters are spatio-temporal structures that change size, effective density and shape constantly (Nikolopoulos et al., 2010). Several empirical and semi-empirical models have been proposed (Gu and Chen, 1998; Harris et al., 2002; Wang et al., 2008; Zou et al., 1994), reflecting the necessity for its accurate prediction. A correlation proposed by Li and Kwauk (1994), based on the work of Chavan and Mashelkar (1980), assumes that the cluster diameter is inversely proportional to the energy used for suspension and transportation. This approach has been widely used by many researchers (Hong et al., 2012; Shah et al., 2011; Yang et al., 2003). However, in some cases those correlations result in