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Numerical investigation of the grid spatial resolution and the anisotropic character of EMMS in CFB multiphase flow

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ABSTRACT

During the last years, considerable efforts have been made for the optimization of numerical methods simulating the operation of the Circulating Fluidized Bed Combustors (CFBC), which imply both the accuracy increase and the computational cost decrease. A foremost goal is the efficient description of its operation under isothermal conditions and the in-depth understanding of the governing complex multiphase flow mechanisms. Grid construction and the calculation of the drag force experienced by the inert material in the two-phase flow are two important parameters for the optimization of the numerical approaches in the case of CFB simulation. The aim of the present investigation is to investigate both the effect of grid density distribution on simulation results and the validity of an anisotropic approach for the drag force calculation through an Energy Minimization Multi-Scale (EMMS) scheme. Grid density distribution is found to affect the numerical accuracy and the real time of simulations. Uniform grid density distribution is found to be the most efficient choice in terms of balance between computational cost and numerical accuracy. On the other hand, EMMS scheme improves the efficiency of detecting complex particle structures (clusters) without an explicit modeling of these spatio-temporal formations. Moreover, applying EMMS scheme only for calculation of the *z*-component of drag force yielded better numerical results compared to a constant interphase momentum exchange coefficient for all the three directions.

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1. Introduction

The technology of Circulating Fluidized Beds (CFB) finds a wide range of applications in engineering processes (Kunii and Levenspiel, 1990; Charitos et al., 2010) and it has therefore been considerably numerically and experimentally investigated in the past decades. Especially in the field of coal combustion, the numerous advantages of Circulating Fluidized Beds Combustion (CFBC), such as fuel flexibility, high boiler efficiency, utilization of by-products and low emissions (Koukouzas et al., 2010, 2011a, 2011b), have led to the construction and the use of large scale units (Wu et al., 2004). For an optimum design of such units, Computational Fluid Dynamics (CFD) models are considered as a powerful tool since they are able to simulate in detail the multiphase flow (gas and solid). Hence, the main endeavor focuses on the development of reliable CFD models, which can with maximum accuracy predict the governing hydrodynamics of CFB reactors by also minimizing the required computational cost.

Except for the grid size and the number of cells, the factors that can directly affect both the computational cost and the numerical accuracy of results also include the grid size distribution. The last decade efforts of many researchers have focused on identifying the importance of the implemented grid type, number and resolution of the computational cells on the numerical results, in the case of CFB modeling (Hartge et al., 2009; Wang et al., 2008a; Armstrong et al., 2010; Lu et al., 2009). There is a variety in the selection of the shape of grid cells reported to have been implemented in the recent literature for such simulations. In the case of cylindrical risers, modeling is carried out either in two-dimensional approaches with the use of squared cells (Wang et al., 2008a; Yang et al. 2003; Tsuo and Gidaspow, 1990; Ibsen et al., 2004) or in three-dimensional approaches with the use of hexahedral unstructured cells (Zhang et al., 2008; Chu and Yu, 2008). On the other hand, in rectangular risers, there is a consensus utilization of hexahedral structured meshes (Hartge et al., 2009; Hansen et al., 2004; Zang and Vander Heyden, 2001; Nikolopoulos et al., 2010a), whilst the relevant distribution of grid nodes is uniform in most of the applications. However, several researchers have tried out to increase the numerical accuracy in

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certain regions of the geometry (dense bed, splash zone, freeboard (De Wilde et al., 2002; Arastoopour, 2001) and side walls (Hansen et al., 2004; Arastoopour et al., 1990)) by implementing denser grids relevant to the other regions. A representative study, which supports the aforementioned statement about the grid density importance on the numerical accuracy, is given by Hansen et al. (2004), which investigated the effect of adding extra gridlines in the bottom zone.

Apart from a well-established mesh, the mathematical formulation and description of the complex multiphase flow is also of high importance for the numerical accuracy. Several numerical approaches have been conducted on the simulation of isothermal flow in CFB reactors, mainly during the last decade (Hartge et al., 2009; Armstrong et al., 2010; Zhang et al., 2008; Zang and Vander Heyden, 2001). In the majority of these studies a Two Fluid Model (TFM, Euler–Euler) is applied for the multiphase flow description (Lu et al., 2009) in contrast to Discrete Particle Model (DPM, Euler–Lagrange), which is not considered to be so efficient in CFB units as in Pulverized Fuel boilers (Ma et al., 2009). For this purpose, various numerical models for the calculation of the drag force between the coupled gas and solid phases are built in order to be implemented in TFM approaches, such as the standard (Wen and Yu, 1966) and the innovative EMMS scheme (Li et al., 2010; Shuai et al., in press a, in press b; Yan et al., 2002). The latter attempts have focused on the elimination of the TFM weakness to assume homogeneous conditions in each cell by taking into consideration the complicated mechanisms of particles clustering in sub-grid level (Wang et al., 2008a; Zang and Vander Heyden, 2001; Nikolopoulos et al., 2010b; Wang and Li, 2007), as far as drag calculations are concerned.

The formulation of the EMMS scheme is not yet well established. On the contrary, its mathematical development, including constraints and assumptions, varies in each analysis (Ma et al., 2009; Nikolopoulos et al., 2010b; Wang and Li, 2007). However, there indeed is a consensus agreement stated in many studies, stating that the effect of the macroscopic heterogeneity of particle structures on drag force calculation in each direction should be taken into consideration. This effect is neglected by most of the standard models such as Gidaspow (1994). Most investigations based on EMMS formulation assume that the correction of a conventional drag force correlation owed to EMMS is constant in every direction (Wang et al., 2008a; Zang and Vander Heyden, 2001; Ma et al., 2009; Nikolopoulos et al., 2010b; Wang and Li, 2007) of the flow field. This is derived from the basic assumption that clusters have a spherical shape inevitably resulting in the notion of symmetrical attitude of drag force in all directions. Thus, according to the abovementioned arguments, the heterogeneity index, calculated based on a one-dimensional approach of multiphase flow, is extrapolated in the calculation of every component of drag force in a three-dimensional simulation, despite the fact that several experimental (Van der Meer, 1997) and numerical (Vashisth and Grace, 2011, Wang et al., 2008b) studies contradict the sphericity of clusters. Therefore, the isotropic approach for the drag force calculation is utilized without having previously examined its range of validity.

It is clear that the mechanism of complex multiphase flow, especially in Circulating Fluidized Beds risers, remains blurred. Probability Density Distribution (PDD) analysis provides several answers about particle movements inside the reactor during a time period, or the way they are distributed in it. For the PDD of transient solid fraction, significant experimental work has been carried out (Zhu and Zhu, 2008; Zhang et al., 2003). However, it should be mentioned that there is no experimental work dealing with the respective spatial distribution. Moreover, it is highly unlikely that such an experimental campaign to be conducted, since the measurement of particles volume fraction in each and every spot of the riser is a sine qua non.

To sum up, the present study in a first step investigates four different grid distributions in a CFB riser keeping constant the total number of grid cells and, in a second step, the application of an alternative EMMS approach. The standard EMMS scheme is compared to an anisotropic one, which turns out to be most suitable in terms of numerical accuracy. Additionally, the distribution of probability density in space and in time is investigated, as an attempt for a better understanding of multiphase flow in CFBs and to enhance the analysis on the volume fraction fluctuations predicted by the two investigated drag models.

2. Grid setup, boundary conditions and implemented models of the numerical simulation

2.1. CFBC pilot unit grid setup

The 1.2 MW riser simulated in the present paper is depicted in Fig. 1. It has an almost 10 m height and a mean cross section (rectangular) equal to around 0.4 m^2. The returning system of the unit is not simulated (Nikolopoulos et al., 2010a); hence, the mean quantity of solids in the furnace is an unknown parameter, which is also not experimentally measured. Both primary and secondary air flow rate and inlet conditions of solid phase are set according to the experimental work of Leithner et al. (1993) under isothermal conditions (825 °C).

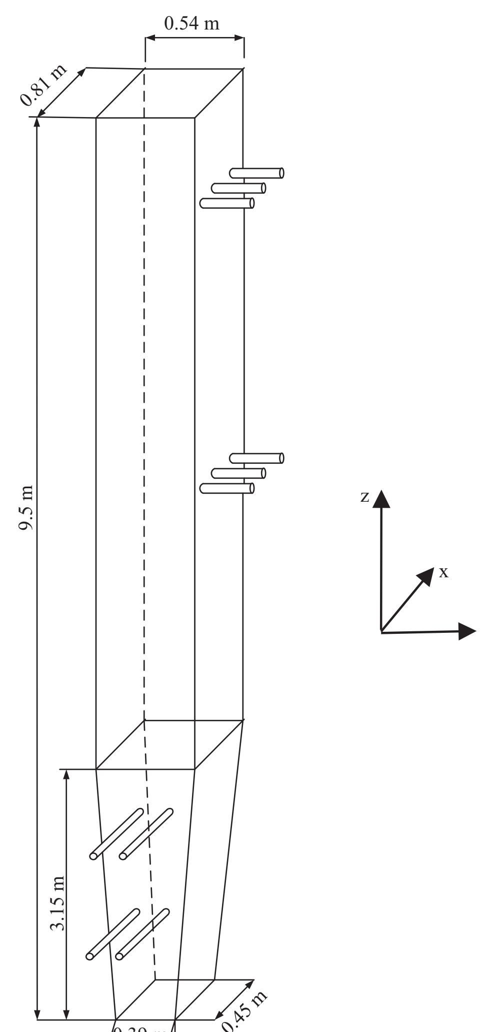

Fig. 1. CFBC pilot plant (Leithner et al., 1993).

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