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Research article

Simulation of the reacting flow within a pilot scale calciner by means of a three phase TFM model

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ABSTRACT

The aim of the present work is the 3-D CFD simulation of the reacting flow inside a pilot-scale calciner, which is part of the 1 MWth dual fluidized bed (DFB) installation located at TU Darmstadt (TUD). The riser of the fluidized-bed calciner is a cylindrical tube with a height of 11.365 m and a varying inner diameter equal to 0.28 m near the bottom area and 0.3967 m at the freeboard. The energy required for the endothermic reaction is provided by the coal combustion inside the same reactor. The gas-sorbent-fuel flow is simulated by means of the pure Eulerian Two-Fluid model (TFM), which is incorporated into the ANSYS Fluent commercial platform, with the implementation of numerous user-defined functions. Owing to the presence of two solid phases a modified version of the Kinetic Theory for Granular Flows (KTFG) for the bi-dispersed flow is applied. The advanced Energy Minimization Multi-Scale (EMMS) scheme with a new cluster correlation and the homogeneous Gidaspow model are applied for the calculation of the gas-sorbent and gas-fuel momentum exchange coefficients, respectively. Additionally, the Syamlal-Obrien symmetric model is used for the calculation of the sorbent-fuel momentum exchange coefficient. Proper reaction rates retrieved from the literature are applied for the simulation of the heterogeneous and homogeneous reactions occurring inside the reactor. Apart from the calcination of $CaCO_3$ to CaO, the carbonation reaction is also incorporated into the numerical model, in order to observe if the reverse reaction is favored, when the temperature is below calcining conditions. The Computational Fluid Dynamics (CFD) model is validated against available experimental data regarding the pressure and temperature distribution along the riser and O_2/CO_2 concentrations at the calciner exit. Simulation results show that the carbonation reaction is indeed favored near the bottom bed, owing to the low temperature values, whilst the calcination rate is equal to zero. Over the height of the burner section, where the fuel enters the reactor, the temperature rises quickly to calcining conditions. Regarding the heat transfer mechanisms, it can be seen that in both solid phases the gas-solid heat exchange coefficient takes its maximum value near the bottom bed and then decreases, as the flow becomes more dilute. This fact reveals the strong dependence between the convective exchange coefficient and the solids volume fraction. Finally, concerning the CFD model accuracy, the different sub-models applied, such as drag-force models, reaction rates, heat transfer coefficients, should be further investigated in future simulations in order to enhance its validity.

1. Introduction

One of the major concerns, nowadays, is the uncontrollable increase in the Earth's temperature that can potentially put in danger the life of the planet. One of the most important contributors to the global warming, which has occurred over the past 50 years, is the carbon dioxide emissions released from power generation, transport and agriculture. One way to reduce the concentration of CO_2, is to capture it before it is released into the atmosphere from power plants and energy intensive industries. The Calcium looping process (CaL) is an emerging post-combustion CO_2 capture technology that is efficient and environmentally friendly. This concept first proposed by Shimizu [1], utilizes a dual fluidized bed system (DFB) that comprises two fluidized bed (FB) reactors, the carbonator and the calciner, which are interconnected by solid transportation lines. In the first reactor, CO_2 from a flue gas is captured by a sand-like (granular material) sorbent – generally limestone or dolomite – whilst in the second reactor the sorbent material is regenerated through a reverse endothermic reaction and fed back to the carbonator unit ready for capture again. In the most common [2] realization of the CaL concept, a pulverized fuel – usually coal – is combusted by oxygen or air inside the calciner, providing, thus, the activation energy of the calcination reaction [3]. In the case of oxy-fired combustion the stream that is produced in the calciner after the sorbent regeneration consists of CO_2 and water vapor. Thus, its main advantage compared to the air-fired combustion is that the CO_2-rich

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stream released is N_2 free and can be easily purified and compressed and subsequently stored in deep geological formations [4]. The present work focuses on the simulation of the three-phase gas-solid flow (gas-sorbent-fuel) inside a pilot-scale FB calciner part of the 1 MWth DFB installation located at Darmstadt University [5], the second largest in the world [6].

Over the last decades, the CaL concept has been tested successfully on the lab and pilot scale ranging from 3 kWth up to 1.7 MWth [7]. The lab-scale activities in facilities, such as the 30 kWth CFB-CFB at INCAR-CSIC [8], the 75 kWth CFB-BFB at CANMET [9], and the 10 kWth CFB-BFB at the University of Stuttgart [10,11], have proven that the calcium looping could be feasible and achieve high CO_2 capture efficiencies. In a European level three pilot scale CaL plants have been constructed; the 1.7 MWth at La Pereda [12] in Spain, the 1 MWth at TU Darmstadt [13], and the 200 kWth at the University of Stuttgart [14]. Following these successful experimental campaigns, attempts are being made, during the recent years, to test the calcium looping concept on the large scale [4,15]. In the context of up-scaling, apart from the experience obtained through the operation of DFB systems on a bench or pilot scale, modelling tools can play a significant role, as well, towards their optimum and effective design. Computational Fluid Dynamic (CFD) models have a strong ability to deliver detailed information concerning the gas-solid flow hydrodynamics occurring inside a fluidized bed unit. Parameters, such as inert material distribution in the bed, particles residence time, reactants mixing efficiency and temperature distribution, can be more easily quantified at any point of the reactor, with a relatively lower cost [16], when compared to the experiments.

In calciner modelling an important aspect that CFD tools can contribute is the optimum reactor design and operation. The accurate simulation of the calciner reactor is a quite essential task, since the calciner is a key component in a CaL system that should operate at a specific temperature range. On the one hand, the temperature should be high enough to push the equilibrium of CO_2 on CaO towards calcining conditions, achieving, thus, effective calcination of the sorbent material and avoiding at the same time its reverse reaction with CO_2 to $CaCO_3$. The necessary heat for the endothermic calcination reaction is provided by combusting several solid fuels and their effective conversion is an important issue that can be also studied in detail using CFD techniques. On the other hand, hot spots and high operating temperatures should be avoided, as sintering [3] might occur. Degradation of the sorbent material can be caused as well due to consecutive carbonation – calcination cycles within the calciner in areas where the carbonation reaction is favored.

Although many papers have been published concerning the CFD simulation of the carbonator unit of the CaL process [17,18], only a few are dealing with the matter of the sorbent regeneration inside the calciner reactor. The literature is even more limited as concerns the coal combustion occurring inside the latter unit. Such task is quite challenging in a sense that along with the flow hydrodynamics, a series of homogeneous/heterogeneous reactions and heat transfer mechanisms should be taken into account. The calciner unit is usually modelled as an oxy-fired reactor operating at temperatures around 900 °C, to ensure complete $CaCO_3$ decomposition [3]. Ylätalo et al. [19] in their work applied two modelling approaches, one 1D dynamic process model and one 3D steady-state model of an oxy-fired calciner model. Atsonios et al. [16] have proposed a new methodology based on the coupling of 3D CFD and advanced 1D thermodynamic models for the simulation of the two-phase (gas-sorbent) flow both in the carbonator and the calciner unit. Apart from these works, however, other similar studies concerning the calciner 3D simulation are not reported in the recent literature. In general, three dimensional simulations are preferable over the two or one dimensional, as they take into account the wall effect and the geometry of the nonsymmetrical flow [20,21].

The most mature methodology for the 3D simulation of the multiphase flow within a FB is the Eulerian-Eulerian Two Fluid Model (TFM) [22]. However, the TFM formulation, which is extended to the Multi-Fluid model (MFM) for the three-phase flow within the calciner, is difficult with a questionable accuracy. The first source of inaccuracy is the scheme applied for the calculation of the drag force coefficient between the primary and the secondary phases. In gas-solid fluidized beds, the interacting phases can potentially form bubbles or clusters of particles depending on the operating conditions and material properties [23]. Such meso-scale structures can affect significantly the underlying physics and reaction mechanisms occurring inside the fluidized bed reactors. The conventional drag force models available in the literature, as that of Gidaspow [24], Syamlal [25] and Wen & Yu [26], assume homogeneous conditions inside a control volume, neglecting, thus, such meso-scale structures. This assumption results in an over-prediction of the drag force induced on the solid particles, especially in cases where a coarse grid is applied. The sub-grid Energy-Minimization-Multi-Scale (EMMS) scheme [27,28], can overcome these problems, by taking into account the clustering formation. A novel extension of this model by [17], which is applied in the present work as well, introduces a cluster correlation that takes into account the riser diameter. However, the main drawback of this EMMS model version, along with other similar versions available in the recent literature, is that it considers that the flow heterogeneity correlates with the mean properties (density, diameter) of the particles flowing inside the reactor, neglecting, thus, the variations in the particle size and density. Recently, a drag scheme of high sophistication encountering heterogeneity in binary mixtures [29] has been developed and could be appropriate for the three-phase flow inside a combusting calciner, as the one modelled in the present work, however it would increase considerably the complexity of the applied numerical model.

The second source of inaccuracy can arise by neglecting the particle size distribution (PSD). Generally, in many industrial-scale CFB applications, such as in calcium looping technology, the bed material is characterized by polydispersity, with a broad PSD [30]. However, the Eulerian simulation of the gas-solid flow hydrodynamics in a CFB unit can be highly demanding in terms of computational cost, when the PSD is taken into account. Thus, it is a common policy, to use a monosized approach, when calculating the solid particles' diameter, with a main drawback that phenomena, such as particle segregation, are neglected [31]. Such phenomena can have a strong effect on flow hydrodynamics and applying a monosized approach can undermine the FB numerical accuracy [28,27,32]. The Multi – Phase Particle – In – Cell (MP-PIC) is an innovative Lagrangian discrete phase methodology (DPM) proposed by [33] that can be used instead of the TFM, because it enables the explicit incorporation of the PSD in the numerical model. Even so, according to [34], the TFM formulation has proven to be highly efficient, due to the application of the kinetic theory of granular flows (KTGF) [35]. An extension of this theory to binary mixtures proposed by CERTH/CPERI [36] based on the work of [37], where more than one solid phases of distinct particle diameters is considered inside the reactor, has been formulated, in a sense that each solid phase is treated as a discrete Eulerian phase. For each solid phase, however, the PSD is not taken into account in order to reduce the computational cost and avoid numerical complexities that arise from PSD incorporation.

A final issue that should be addressed is the calcination reaction mechanisms. Contrary to the flow hydrodynamics simulations, the understanding of the sorbent regeneration, has been the subject of many research studies [38]. Unfortunately the quantification of the calcination kinetics is a really complicated issue, because the reaction itself is highly dependent on the CO_2 partial pressure and the particle size, whilst it can be inhibited by impurities, such as fly ash [39,40]. As regards the calcination kinetics a series of reaction rates have been presented in the literature. The dominant models proposed regarding the specific surface area quantification are the Shrinking Core Model (SCM) [41,42] and the Changing Grain Size Model (CGSM) [38]. Garcia-Labiano based on these models proposed a particle model for the most usual calcium based-sorbents for a wide range of operating conditions [38]. Apart