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CFD modelling of CO_2 enhanced gasification of coal in a pressurized circulating fluidized bed reactor

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ABSTRACT

Two CFD models of CO_2-enhanced coal gasification in pressurized circulating fluidized bed reactor were developed and applied to simulate the process and predict syngas composition at the reactor outlet. The models were developed using commercial codes ANSYS Fluent and CPFD Barracuda. The models allowed to predict the outlet syngas composition and give insight into the processes occurring in the reactor. Results of the analyses were compared with experimental data obtained from a small scale test facility. The predicted syngas compositions agreed well with the experimental data, however the local gas composition in some instances were different. The predicted temperature distribution in Fluent agreed well with the experimental data. The examined cases confirmed that addition of CO_2 to the gasifying agent in a pressurized reactor can increase the CO yield per unit of feedstock and reduce the oxygen demand.

1. Introduction

Gasification is a thermo-chemical conversion process of carbonaceous feedstock into gaseous product called syngas. The syngas is composed mostly of CO and H_2. It can be used for electricity and/or heat generation or as a feedstock for production of hydrogen, methanol, gasoline or other substances. Gasification of solid fuels is realized in fixed (moving), entrained flow and fluidized bed gasifiers. The fluidized bed (FB) gasifiers are characterized by high efficiency and availability, good fuel flexibility, long residence times of fuel particles in the reactor, high mass and heat transfer rates between the gaseous and solid phase [1,2] and acceptance of large fuel particles. These features allow for using versatile feedstocks for syngas production, which include: bituminous and sub-bituminous coals, coke, low rank coals, lignites and biomass [2,3]. Gasification in fluidized beds is realized at low temperatures (typically 800–950 °C, up to 1100 °C for agglomerating gasifiers), when compared to the entrained flow gasifiers. The low temperature is required due to the need for maintaining the ash in solid state. Typically oxygen, air or oxygen/steam and air/steam mixtures are used as gasifying agents. However, utilization of CO_2 as an additive to the gasifying agent is interesting due to the carbon and oxygen carried in the CO_2 stream. If the carbonaceous feedstock can be converted by means of CO_2 to produce CO through the Boudouard reaction, the process efficiency can be increased due to increased chemical enthalpy flux of syngas, reduced expensive oxygen consumption and reduced relative CO_2 emission [4]. The energy required by the endothermic Boudouard reaction could be covered by the smaller heat production or in an adiabatic case by the exothermic reactions. The concept of using CO_2 as a gasifying agent is not new and the state of the art was described in a review paper [5]. It was shown in Ref. [6] through thermodynamic calculations, that addition of CO_2 to the gasifying agent can lead to substantial decrease of feedstock consumption at the same CO production, when compared to conventional (without CO_2 addition) gasification. It should however be stressed that the reaction rates of chars with CO_2 are several orders of magnitude lower than with O_2 [7]. This limits the carbon conversion rate and production of large amounts of CO through the Boudouard reaction. The carbon conversion rate in CO_2 atmosphere can be increased by increase of pressure [5,6], and by increase of process temperature [5]. The latter however is limited in fluidized beds due to the requirement of process temperature to be below the ash fusion temperature. A potential to increase the conversion rate was also observed during co-gasification of coal with biomass. The alkali and alkali earth metals present in biomass act as catalyst during co-gasification

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[8–10]. Application of pressurized fluidized bed reactors for gasification is a perspective technology due to possibility of reduction of investment and operation costs, and recent improvement of availability of this technology [4].

The most frequently used approaches to CFD modelling of particle laden flows and in particular the hydrodynamics of circulating fluidized are the meso-scale methods. Spatial scales covered by these methods range from particle sizes to the sizes of the modelled device [11]. The meso-scale methods include the well-established Eulerian-Eulerian (EE) approach, in which the gaseous and solid phases are treated as interpenetrating continua, and the Eulerian-Lagrangian (EL) models, in which the gaseous phase is treated as continuous and the solid phase as discrete. An advantage of the EL approach is that the particle size distribution is naturally included. In the EE approach additional effort of modelling multiple phases or using the moment methods [12] is required. It should be stressed that in the Eulerian-Lagrangian models individual particles or their groups (clouds, parcels) can be tracked in the Lagrangian frame of reference. This feature allows to considerably reduce the computational effort, and therefore systems containing large numbers of particles, such as those occurring in pilot and industrial scale units, can be simulated [13–15].

A particularly difficult aspect of the EL approaches is appropriate modelling of particle-particle interactions [16,17]. Another challenge is to extend the models to include reacting flows, which would allow them to be used for modelling of reactors and boilers. The various approaches and applications in this context were presented in recent review papers [2,18] and thus the readers are directed to these publications. Additional more recent publication of Kraft et al. [19] focuses on modelling of large scale dual fluidized bed biomass gasifier. In this study steam was used as the gasifying agent. The authors obtained good agreement between predicted and measured syngas composition, and indicated that the best solids recirculation rate was obtained for the EMMS drag model. The EMMS model allows for taking into account the heterogeneity of the particles in the flow. The same finding was reported in Ref. [20] in which hydrodynamics of a complex full-loop CFB was studied.

According to the best knowledge of the authors there is only one study of Cheng et al. [21], where numerical analysis of CO_2-enhanced gasification in fluidized bed reactor is presented. The authors used the EE approach for modelling of biomass gasification.

The Eulerian-Lagrangian models, were implemented in several open source, e.g. MFIX, and commercial codes e.g. ANSYS Fluent and CPFD Barracuda. Although they differ in several aspects, which include the way the particle-particle interactions are computed, the principal approach of tracking of particle parcels is the same. In ANSYS Fluent a discrete phase model (DPM) for dilute systems was extended by application of the kinetic theory of granular flow (KTGF) to account for the particle-particle interactions [22–24]. In the CPFD Barracuda code the MP-PIC method is used [25–28].

In this paper two CFD models for simulation of CO_2-enhanced coal gasification in a pressurized circulating fluidized bed (CFB) reactor are presented. The models were developed using two commercial codes; the ANSYS Fluent and the CPFD Barracuda. The objective of the study was to verify the ability of the models developed in two CFD codes to predict the CO_2-enhanced gasification process. The methodologies applied in this study were based on previously developed models [28,29]. Several improvements, however, were introduced and described. In both cases the Eulerian-Lagrangian approaches were used. Three case studies are presented in which simulation results in terms of syngas composition and temperature distribution are compared with experimental data. The experimental data were obtained from a small scale gasification reactor.

2. The gasification reactor

The gasification reactor under consideration is a pressurized circulating fluidized bed reactor built and tested at the Clean Coal Technologies Center of the Institute for Chemical Processing of Coal in Poland. A photo and a schematic diagram of the installation are presented in Figs. 1 and 2, respectively.

As presented in Fig. 2, the coal is fed to the reactor (9) with a screw feeder (4). The gasification process can be carried out at temperatures up to 1000 °C and pressures up to 1.5 MPa. The maximum reactor capacity is 100 kg/h of coal. The process gas is discharged from the reactor via the riser (10). The gas leaving the reactor contains char particles and other particulate matter. Thus, the gas is directed to particulate matter removal unit. First, the char is separated from syngas in the primary cyclone (11). The particles of char fall into the recycling tank (13), from which they are returned to the reactor (char recycling). Part of the char, as one of the two main products of the process, is being discharged from the system to char tank (17). After the char removal the gas is deducted in a cyclone (15) from which solid particles are directed to a tank (17). The last stage of gas deducting takes place in a ceramic filter (19), from which purified gas is directed to water scrubber (21), where it is cooled and at the same time tar compounds are removed. After the scrubber, the gas is cooled down in a heat exchanger (24) and then desulphurised and dehydrated in adsorbers (27). Such prepared process gas is directed, depending on the needs, to other experimental installations, where alternative processes of its purification and conversion are examined. The excess gas is burnt in a combustion chamber (30) [30]. Geometry of the reactor used to build the numerical model is presented in Fig. 3. The reactor encompasses a barrel like bottom part, in which strong internal recirculation of the solid phase develops, and a riser section, which is connected to a separator (not shown in the figure). As mentioned earlier, the separated solids (char, sand and ash) can be recirculated to the bottom, barrel like part of the reactor through a loop seal (not shown in the figure) and through a recirculation inlet, however in the investigated cases they were not. The coal was introduced through a circular inlet at the side of the bottom barrel part. The inlet has the same diameter and is placed at the same

Fig. 1. The experimental facility at the Institute for Chemical Processing of Coal.