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Research article

Numerical and experimental study of heavy oil gasification in an entrained-flow reactor and the impact of the burner concept

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ABSTRACT

This work studies the heavy oil gasification experimentally and numerically. The experimental investigations use the semi-industrial test facility HP POX (High Pressure Partial Oxidation gasifier), operated at the Institute of Energy Process Engineering and Chemical Engineering, TU Bergakademie Freiberg. The HP-POX facility with a capacity of 5 MW operates under industrial conditions and features comprehensive instrumentation. The numerical model considers state-of-the-art model approaches and a detailed determination of the droplet size distribution, applying breakup models to the liquid heavy oil phase. The optical system of the HP-POX allows the heavy oil injection to be observed; these observations are then used to evaluate the droplet size distribution. The numerical model approach is validated against two lab-scale experiments from the literature, which also provide data on high pressure and temperature conditions. Validation A is the pressurized entrained-flow reactor of the Commonwealth Scientific and Industrial Research Organisation applying coal gasification at 20 bar. Validation B is the research gasifier for liquid fuel, of the Central Research Institute of Electric Power Industry that gasifies Orimusion® at 19 bar. The numerical model shows good agreement for both experiments, and for the heavy oil gasification experiment in the HP-POX plant. The validated model is used to study the impact of two different burner concepts on gasification characteristics. Burner 1 has a central fuel injection and an annular gasification agent injection, while Burner 2 has a central gasification agent injection and an annular fuel injection. The results show that Burner 1 achieves a higher syngas yield (H_2 + CO) but with higher soot production in comparison to the simulation results for Burner 2.

1. Introduction

The gasification of heavy hydrocarbon feedstocks is considered as a valuable source of producing syngas (H_2 + CO) and hydrogen for the chemical industry and refineries [1–3]. Essential requirements are a high syngas quality yield for further synthesis, to have less remaining char and soot formation, and to minimize gasification agents in order to reduce the operating costs.

Fuels for heavy oil gasification can be heavy or extra-heavy crude oils, and atmospheric and vacuum residues of distillation in refineries. To upgrade the feedstock, catalytic processes (such as residue fluid catalytic cracking (RFCC), and catalytic cracking in a fluidized bed reactor (FBR)) and thermal processes (such as solvent deasphalting (SDA), gasification, visbreaking, delayed coking, fluidcoking, flexicoking) can be used. Catalytic processes are not robust against the rising metal contents (≈1000 ppm Ni + V) and rising coke-forming tendencies (Conradson Carbon) of the current heavy crude oils [4]. Hence, the thermal processes gasification is a valuable option; here entrained-flow gasification technologies such as AirLiquide Multi Purpose Gasification, Texaco/GE Gasification or the Shell Gasification Process can be applied [1,5-8].

The usage of numerical models is one method to gain a better understanding of the various phenomena and to develop improved technologies based on this findings, which is discussed in this work. The gasification of heavy oils is a multi-scale process that is complex to model. Few multi-dimensional gasifier models for hydrocarbon feedstocks are available in the literature [9–11], and these are only validated for their respective gasification cases. Hence, the model approach applied here is validated against two gasification experiments from the literature and against one in-house experiment, to achieve simulation results which are reliable as possible.

Moreover, to simulate the gasification process it is essential to appropriately model the mixture of the gas phase and the liquid phase. The model discussed here focuses on the liquid fuel injection, as the atomization of the highly viscous liquids and the mixing with the gasification agents are critical issues that limit the conversion rate. The

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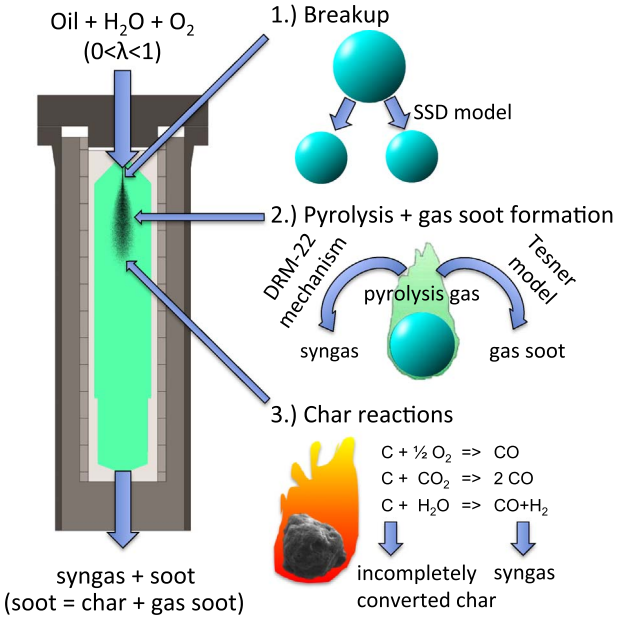

Fig. 1. Schematic overview of the heavy oil gasification process.

conversion rate is basically determined by the heat and mass transfer between the resulting droplets and the gas phase, which highly depends on the droplet size. Since the droplet size distribution is essential, this work is focused to estimate the droplet size distribution with a sufficient precision as possible. For that reason, a separate spray experiment is conducted in the HP-POX test facility to determine an appropriate droplet size distribution.

Finally, the validated overall model approach, with the adjusted droplet size distribution, is used in this work to study the impact of different burner concepts on the fuel conversion and soot production.

2. Numerical model

2.1. Modeling approach

Fig. 1 illustrates the general model approach for the heavy oil gasification. The gasifier is modeled as a two-dimensional axis symmetric reaction chamber.

The conversion process starts with the injection of the liquid fuel and the gasification agents. The discrete phase (droplets/char) are modeled as Lagrange particles in a discrete particle model (DPM) framework. The release of the volatile matter of the heavy oil is described using droplet models in combination with additional pyrolysis approaches, which are discussed in more detail in the following sections. The gas phase is modeled using the Eulerian approach and is assumed to be an incompressible ideal gas. Buoyancy effects are taken into account.

The turbulence is modeled using the k-ω-SST approach. The interaction between the discrete phase and the gas phase is considered by two-way coupling. The turbulent dispersion of the particle path-ways is represented using the discrete random walk model, which is a stochastic particle tracking model. The reaction rates of the gas phase are determined with the DRM-22 [12] reaction mechanism. The eddy-dissipation concept is used for turbulence-chemistry interaction. Radiation is considered using the P-1 model, applying the weighted-sum-of-gray-gas model for the absorption coefficient of the gas species. The emission coefficient of the particles is assumed to be unity [13].

The heat capacities of the individual gas species are determined using the polynomial property function with the coefficients given in [13,14]. The thermal conductivity and the viscosity of the individual gas species are estimated using kinetic theory. The thermodynamic properties of the mixture are modeled applying the mass-weighted-mixing law. All thermodynamic properties of the discrete phase are assumed to be constant. The pressure-velocity coupling is solved with the coupled scheme. The convective terms of the governing equations are discretized with the QUICK scheme. The software ANSYS® Fluent 17.2 is used to solve the above-mentioned governing equations.

2.2. Droplet breakup

The fuel atomization depends on injection parameters such as the relative velocity between liquid and gas, the liquid and gas densities, and the liquid viscosity and surface tension. The breakup of the liquid phase can be divided into a primary and a secondary breakup. The primary breakup occurs at the nozzle tip and is caused by the dynamic pressure release when the fuel-steam mixture is injected into the gasifier. The subsequent atomization of the individual droplets and ligaments is called secondary breakup and is caused by shearing forces between the droplets and the surrounding gas flow. The shear stress increases with high relative velocities between the liquid fuel and the gas phase, and is decreased by a high liquid viscosity and a high surface tension.

The secondary breakup of the heavy oil droplets is modeled using the Stochastic Secondary Droplet (SSD) model [15], which determines droplet size distribution by considering the breakup as a discrete random event. The breakup model describes when and how many child droplets are created. The SSD model requires three model parameters, which are We_{cr}, C and ξ and are set to 6, 1.73 and -0.1 respectively, as suggested by [13]. Their usage is shown in the following. If the droplets are larger than a critical droplet diameter, $d_{p,c}$, then these are subjected to breakup. The critical droplet diameter is determined with

$$d_{p,cr} = 2\frac{We_{cr}\sigma_l}{\rho_g u_{rel}^2}, \tag{1}$$

and considering the critical Weber number, We_{cr}. The properties of the liquid phase are indicated with the subscript l, those of the gas phase with g, and in general the discrete particle properties with the subscript p. The relative velocity difference between the two phases is given with u_{rel} and the surface tension with σ. The breakup occurs only if the breakup time, t_{bu}, is reached, which considers C and reads

$$t_{bu} = C\sqrt{\frac{\rho_l}{\rho_g}}\frac{r}{|u_{rel}|}, \tag{2}$$

with ρ as the density. The diameter of the child droplets is obtained from the size distribution function, F, which considers the SSD model parameter ξ and reads

$$F = \frac{1}{\sqrt{2\pi\xi^2}}\exp\left(\frac{-\left(\ln\left(\frac{d_p}{2}\right)-\ln\left(\frac{d_{p,0}}{2}\right)-\xi\right)^2}{2\xi^2}\right). \tag{3}$$

2.3. Pyrolysis

After the droplet is heated up sufficiently, it is assumed to release volatile matter and to form a solid char from the remaining matter. The volatiles, including tar, are modeled as gas species and the char as pure carbon. The pyrolysis model describes the conversion rate, the species composition of the volatile matter, and the amount of volatile and char matter. The pyrolysis model starts when the particle temperature reaches vaporization temperature and is active as long as volatile matter remains. The particle temperature can only heat up until an assumed maximum pyrolysis temperature during the volatile matter release.

In this work, the applied rate of the change in particle mass m_p over time t during the pyrolysis is described by [16] and is combined with a

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