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Deposition and slagging in an entrained-flow gasifier with focus on heat transfer, reactor design and flow dynamics with SPH

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ABSTRACT

Two different types of coal are evaluated in a generic gasifier. The gas and discrete phase in a gasifying process was computed in ANSYS Fluent to determine particle trajectories and deposition rates at the wall. This information serves as input for the slagging tool developed by the authors to simultaneously compute the processes of deposit built-up and slag flow. The tool utilizes the method SPH (Smoothed Particle Hydrodynamics), and due to the particle nature of this method, each particle representing the slag gets its own physical properties such as viscosity or thermal conductivity. Thus the slag's surface and interfaces between solid and liquid layers can be determined without problems. The tool detects critical parts in the gasifier that show increased slag deposit and determines the thickness, temperature profile, and particle distribution of the slag layer. One Puertollano coal and one Colombian coal are evaluated in terms of their slagging propensities, which show different behavior in deposition build-up and flow dynamics. Areas with a low amount of slag matter inside the deposit produce an insulating effect, which changes the physical properties of the slag layer. Predicting the slagging propensities of different types of coal using data acquired from slag simulations can support the gasifier design process.

1. Introduction

Slagging can lead to shut-downs and reactor damage in high-temperature gasification processes. Although a slag layer is desired to a certain extent at the walls to prevent corrosion, too much slagging prevents heat transfer through the membrane walls, restricts the flue-gas path, and moreover results in falling solid-slag debris that can destroy parts of the reactor. Maintenance is costly, therefore it is of upmost interest to gather enough information about the coal ash's effect on the reactor under specific operation conditions to reduce the harmful impact of slagging. Coal-ash composition, critical temperatures, and other indices can yield a first prediction about how slag will behave during gasification. Designing a complete reactor is normally focused on fulfilling the specific requirements of the coal sort in terms of slagging propensities to ensure a stable process. But due to a more flexible world market, nowadays not only the coal sort is used the gasification reactor is designed for. Also coals with completely different compositions and thus varying physical and chemical properties are utilized. Although slagging indices deliver a first hint about the extent to which the reactor will be affected, no information about operating conditions such as temperature and pressure, the specific geometry of the walls and heat-transfer surfaces, the type of reactor, and the flow behavior of the slag is given. Simulations can help to bridge the gap between rough estimates of slagging propensities and the actual conditions during the gasification process.

One of the earliest slag models was created by Reid and Cohen [5] for a slag-tap furnace with parameters such as viscosity, surface temperature, slope of the wall and slag volume. Based on these principles, other models and improvements were implemented by [6,19,20], who simulated different reactor configurations. Here the model of Seggiani [20] is important to mention, since it influenced a large number of current developments [2,24,25]. Other authors have implemented models for deposition and wall burning, among them [15,21,23]. These mechanisms can be implemented in the existing models for the slag flow. All of the slag flow models use an analytical cell-based method. A disadvantage of this approach is the beforehand given temperature profile and a computed flow velocity based on viscosity, slope, and distance to the walls. No detailed insight into the flow and deposition dynamics can be obtained.

Unlike most simulations that take a cell-balance approach with a given temperature gradient through a solid and liquid slag layer having a boundary predescribed by the temperature of critical viscosity to determine the slag thickness in every cell, Computational Fluid Dynamics (CFD) simulations can yield insight into the processes of deposition and slag flow. Ni [16] performed one of the earliest CFD simulations using the commercial software package FLUENT and its volume-of-fluid model to simulate slag flow. The results were compared with those from cell-based models. Another FLUENT simulation was done by Chen [3], with a discrete phase for the deposition process and a

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volume-of-fluid model for multiphase interaction. The volume-of-fluid approach has drawbacks in representing free surfaces, phase boundaries and break-ups of the slag layer. To overcome these drawbacks, the method in this work represents the slag matter as interacting particles for modeling and simulating deposition and slag flow. This approach is called SPH (Smoothed Particle Hydrodynamics) and the software tool developed by the authors utilizing this method is first used in the work of Kurowski and Spliethoff [7]. The tool allows the slag layer's initial build-up to be followed to identify critical points in the reactor as well as the flow of the liquid part and its interaction with the solid part of the slag. Due to the particle nature of the simulation method, mechanisms like deposition, solidification, heat transfer, and flow dynamics can be implemented and analyzed to find optimal operating conditions for the gasification process. A short explanation of SPH is provided below.

2. Introduction to SPH

SPH is a Lagrangian particle method as opposed to continuous Euler methods; no mesh for discretization is needed. Therefore the domain is discretized by particles that interact with each other. Based on this interaction, resulting forces are generated. The forces act on the particles creating movement. To find the strength of the interaction between two particles, an integral function is used [12]:

$$A(x) = \int A(x\prime)\delta(x-x\prime)dx\prime \tag{1}$$

Here, A is an unknown physical value at position x. It depends on A at position x' and the Dirac function $\delta(x-x')$. The Dirac function has a value of 1, if $x=x'$, otherwise it is 0. The integral function of Eq. (1) can be approximated by [12]:

$$A(x) = \int A(x\prime)W(x-x\prime,h)dx\prime \tag{2}$$

The smoothing function $W(x-x',h)$ is calculated within a specific range given by h. This function samples the particle number density, therefore it has the dimension of an inverse volume.

An approximation valid for particles is needed when considering particle interaction. Replacing dx' with δV (the volume of a particle), and with $\delta V = m/\rho$ (mass and density of a particle, respectively), Eq. (2) can be written as [14]:

$$A(x_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} A(x_j) W(x_i - x_j, h) \tag{3}$$

The indices i and j indicate specific particles. N gives the total number of particles in the domain. In the following, $W(x_i-x_j,h)$ will be replaced by the short form of W_{ij}.

The derivative of the particle approximation is applied to the smoothing function, and therefore [14]:

$$\nabla A(x_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} A(x_j) \nabla W(x_i - x_j, h) \tag{4}$$

2.1. Density approximation

Density in SPH is approximated according to the Navier-Stokes continuity equation. A possible way to approximate density is [13]:

$$\frac{\partial \rho_i}{\partial t} = \sum_{j=1}^{N} m_j v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}} \tag{5}$$

Here, β is the respective spatial coordinate direction. This approximation delivers good results close to boundaries and interfaces.

2.2. Momentum approximation

The particle approximation of momentum, which also considers symmetry for radial and normal momentum, can be written as [8,13]

$$\frac{\partial v_i^{\alpha}}{\partial t} = \sum_{j=1}^{N} m_j \left(\frac{\sigma_i^{\alpha\beta}}{\rho_i^2} + \frac{\sigma_j^{\alpha\beta}}{\rho_j^2} \right) \frac{\partial W_{ij}}{\partial x_i^{\beta}} + F_i \tag{6}$$

F_i represents body forces such as gravity; σ is the total stress tensor comprising one part for volume change and one part for viscous stress. The coordinate directions are given by α and β. v is the velocity of a particle.

2.3. Energy approximation

The approximation of energy contains the total stress tensor from Eq. (6). With the process of heat conduction, the complete energy equation is given as [4,8]:

$$\frac{\partial u_i}{\partial t} = \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) v_{ij}^{\beta} \frac{\partial W_{ij}}{\partial x_i^{\beta}} + \sum_{j=1}^{N} \frac{4 m_j}{\rho_i \rho_j} \frac{k_i K_j}{k_i + k_j} (T_i - T_j) \frac{\partial W_{ij}}{\partial x_i^{\beta}} + \frac{\mu_i}{2\rho_i} \epsilon_i^{\alpha\beta} \epsilon_i^{\alpha\beta} \tag{7}$$

Internal energy is represented by u, the pressure is given by p, k is the thermal conductivity, μ the viscosity and T the temperature value of a particle. The shear rate is indicated with ε.

3. Slag modeling

Originally applied to hydromechanics, SPH needs adjustments to enable it to simulate the slag flow of coal ash in gasifiers. These adjustments are of a numerical as well as a physical nature. A faster search algorithm and code parallelization was implemented to deal with a large number of particles when simulating a complete gasifier.

3.1. Physical properties of slag

All physical properties are calculated based on the composition of coal ash oxides. Therefore different coal sorts can be compared to each other. The slag density is computed using the partial molar volumes approach [10]:

$$V = x_1 \overline{V}_1 + x_2 \overline{V}_2 + x_3 \overline{V}_3 \ldots \tag{8}$$

$$\rho = (M_1 x_1 + M_2 x_2 + M_3 x_3 + \ldots)/V \tag{9}$$

The partial molar volume of component i is given by $\overline{V}_i$, the molar mass and weight by x_i and M_i, respectively, and V is the total molar volume. The density from Eq. (9) is the initial density of the slag particles.

Similar to the density approach, the model for heat capacity of the slag utilizes the partial molar heat capacities, based on [11]:

$$C_p = x_1 \overline{C}_{p1} + x_2 \overline{C}_{p2} + x_3 \overline{C}_{p3} + \ldots \tag{10}$$

The partial molar heat capacity of component i is given by $\overline{C}_{pi}$, and $\overline{C}_p$ is the total heat capacity of the slag. This value is needed for the thermal conductivity. Thermal conductivity can be calculated with the following equation [11]:

$$k_{\text{eff}} = a_{\text{eff}} C_p \rho \tag{11}$$

Here k_{eff} denotes the thermal conductivity, and a_{eff} is the thermal diffusivity, based on experimental data.