Full Length Article

Modeling of ash deposition on the wall of a high temperature slagging gasifier

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ABSTRACT

In high temperature gasification reactors, inert ashes coming with the feedstock deposit on the walls in the form of slag. In these kind of reactors, external cooling screens are used to control slag deposition. A transient 2D model was developed and implemented to simulate the growth of a slag liquid-solid layer at the walls of an entrained flow coal gasifier operating at 1200–1500 °C and external cooling at 30–600 °C The model results were compared with those of other models present in the literature. The effect of operating variables on layer thickness and wall heat flux were studied through sensitivity analysis. The study shows that the most important parameter controlling slag accumulation is the difference between gas temperature and slag critical viscosity temperature. This affects slag viscosity and eventually the degree of wall agglomeration at steady state. The role of the external cooling temperature and ash flowrate was also investigated. The model was modified to account for the effect of gas cooling due to wall heat transfer by convection and radiation. Results show that if gas flowrate is low, e.g. a small-scale unit, this effect is not negligible, contrarily to what is usually assumed in the literature.

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1. Introduction

Gasification is an important technology for the conversion of solid hydrocarbons (coal and/or biomass) into valuable syngas. This intermediate product is used in a number of important applications, from synthesis of liquid fuels (Fischer-Tropsch process), to methanol [1]. Besides, it can be used in combined heat and power applications [2].

The main product of gasification is a mixture of gases called syngas (H_2 and CO mainly, with a variable content of CO_2 and CH_4). Important by-products are tars (hydrocarbons that are condensable at room temperature), char (solid carbonaceous species with very low hydrogen content), and ashes, a mixture of inorganic compounds (mainly metal oxides) that are originally present in the feedstock and cannot be further converted. In general, the target is to maximize gas yields. Some studies about catalytic conversion of tars at relatively low temperatures show promising results [3]. Nevertheless, kinetics for gas phase conversion of tars and char are known to be quite slower than those of the original biomass at low temperatures [4]. Alternatively, high temperatures (>1300 °C) are needed to carry out thermal conversion of tar and char at a reasonably low residence time, to avoid the need of very

big reactor volumes. This temperature is usually higher than the melting point of ashes. So if high temperature gasification is carried out, partial or total melting of ashes is expected. This can lead to a number of problems in the reactor operation. Molten slag can easily stick to the reactor walls, and the inlet and outlet pipes. Its accumulation can possibly lead to clogging if not properly controlled. Liquid slag can also be chemically active at high temperatures, leading to leaching of the refractory walls when permanently in contact with it. As a result, the lifetime of the walls' material is decreased to a few months [5,6]. As a consequence, slag control is one of the main issues in a high temperature gasifier. One possible way to address these problems is to use the slag itself as a refractory layer at the walls [7–9]. Layer growth can be controlled by applying external cooling, thus setting the heat flux at the walls [10]. The deposited solidified slag has an insulation effect because of the low thermal conductivity of the metal oxides composing it. After some time, the system reaches an equilibrium so that the inner temperature is high enough to avoid solidification of the new liquid slag, which flows downwards after being deposited on the solid layer [11]. From that moment on, the layer does not grow any more. Final thickness depends on the properties of the slag and the operating conditions of the reactor and must be estimated when designing the reactor, ensuring that no clogs are formed.

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Nomenclature

$Cp\ Cp_g$	heat capacity of slag and gas (J/kg/K)
C_d	drag coefficient (–)
g	gravitational acceleration (m/s^2)
$h_g\ h_w$	gas-liquid and solid-wall heat transfer coefficients (W/m^2/K)
j_s	slag mass flux at gas-liquid interface (kg/m^2/s)
K_{gl}	momentum transfer coefficient (Pa m/s)
k	slag thermal conductivity (W/m/K)
$\dot{m}_{dep}$	slag flowrate (kg/s)
$\dot{m}_g$	gas flowrate (kg/s)
n	normal coordinate to the boundary surface
$q_{rad}\ q_{cnv}\ q_{dep}$	heat fluxes due to radiation, convection, and slag deposition (W/m^2)
R	reactor radius (m)
r	radial coordinate (m)
$T\ T_g\ T_w$	temperature of slag, gas, and cooling water (K)

$u_r\ u_z$	radial and axial velocity components in cylindrical coordinates (m/s)
$u_n\ u_t$	normal and tangential components of velocity at boundary (m/s)
u_t^g	gas velocity (m/s)
V_s	slag volume (m^3)
z	axial coordinate (m)
$\delta\ \delta_L\ \delta_S$	slag thickness, total, of liquid and solid layer (m)
ε_s	slag emissivity (–)
μ	slag viscosity (Pa s)
ρ_s	slag density (kg/m^3)
σ	Stefan-Boltzmann constant (W/m^2/K^4)
$\tau_{rr}\ \tau_{zz}\ \tau_{rz}$	components of 2D stress tensor in cylindrical coordinates (Pa)
$\tau_{nn}\ \tau_{nt}$	normal and tangential component of boundary stress (Pa)

A first analytical model describing the slag flow was proposed by Seggiani [12]. The latter is quite simple and can predict the behaviour of different gasifiers with a reasonable degree of confidence. Some simplifications were made on the temperature profile, allowing analytical integration of the 1D momentum equation. More detailed approximations of the temperature profile were introduced by Kittel et al. [13], and Yong et al. [14]. Ye and Ryu developed a fully numerical model solving the momentum and energy equations inside the slag layer, using a finite volume approximation and a dynamic addition of control volumes [15,16]. Their model fairly compared with the results obtained by Seggiani [12] and Yong [14]. Yang et al. [17] applied Seggiani's model to a reactor network model (a set of PFR and CSTR in series and in parallel to approximate the reactor fluid dynamics), to couple the description of the slag film with the reacting gas. More recently, Chen and Ghoniem extended the application to a CFD model [18] to describe the local deposition of slag in a complex reactor geometry using a Volume of Fluid approach.

A key aspect to correctly describe slag behaviour can be directly correlated to an adequate characterization of slag properties, in particular its viscosity as a function of temperature [9,19]. Since both solid and liquid slag are present in the system, phase transition must be correctly addressed. Such transition is usually not sharp (ashes are generally a mixture of chemical species with different melting points), and a temperature range in which the material is progressively softened can be defined. This range can be specified by performing standard ash fusion tests. The most important one is the cone test (e.g. ASTM D1857 [20]), which is performed by placing cone ash samples in an oven and observing their deformation at different temperatures. Four temperatures are defined based upon the shape of the deformed cone (initial deformation, softening, hemispherical and fluid). Within this range, a change of the rheological behaviour can usually be observed. A critical viscosity temperature (T_{cv}) can be defined, above which slag behaves like a Newtonian fluid and can be considered as a liquid with a viscosity exponentially decreasing with temperature. The critical viscosity temperature is linked to the ash melting points. Some authors tried to correlate T_{cv} with the softening temperature [21,22], or the hemispherical temperature [23], while Song et al. [24] proposed a function of the liquidus temperature of the material, calculated with a thermodynamic software. Some examples of melting temperatures measured for coal, synthetic and biomass ashes are shown in Table 1.

In general, T_{cv} depends on the chemical composition of the ash [29,30], so it is a representative parameter of a system operating with a certain type of feedstock. Some synthetic indicators used to correlate this parameter with composition are the base-to-acid ratio [31,30], or the Q factor (related to the degree of polymerization of the molecular chains [29]). A lot of research has been done in the years to characterize the viscosity of slags. One of the earliest correlations by Hoy et al. [32] assumes a dependency on the square of the Silica factor. The matching of experimental data was improved by Watt and Fereday [33], who introduced an Arrhenius dependency of viscosity on temperature, with both activation energy and pre-exponential factor as a linear combination of the amount of SiO_2, Al_2O_3, Fe_2O_3, CaO and MgO. A quite widely used correlation was introduced by Urbain [34], who extended the theoretical approach by Weymann [35] and proposed an exponential law, with two parameters depending on the fraction of three group species (glass formers, amphoterics and modifiers). The Urbain model was extended and modified by several authors. Riboud and Larrecq [36] changed the equation parameters, introducing polynomial functions of the composition. Other variations were proposed by Kondratiev and Jak [37], Frank and Kalmanovitch [38], Streeter et al. [39], Mudersbach et al. [40]. A compared analysis of different models by Vargas et al. [41] on different types of coal ash showed that while the Urbain model leads to generally satisfactory results compared to experimental data, the Frank and Kalmanovitch has better prediction of slag viscosity for slags with high silica content. A different correction to the Urbain model was proposed by Mills and Sridhar [42], who introduced a function of the optical basicity, which better quantifies the degree of depolymerisation. Other authors calculate the parameters from thermodynamics [43,44]. Different types of model may include a function of the concentration of solid crystals [45] (particularly suitable when temperature is close to the T_{cv}), and the application to non-Newtonian fluid models [46]. More comprehensive reviews of the main constitutive models for slag viscosity and other transport properties are reported elsewhere [29,47–49].

In the present study, a detailed time-dependent 2D model to describe slag flow is presented and discussed. The model results were then compared with the main ones found in literature models for a given base case, and the main variables controlling the sensitivity of the model were identified. A model refinement was also proposed to account for gas cooling due to heat transfer with the slag at the wall.