Modeling the slag layer in solid fuel gasification and combustion – Formulation and sensitivity analysis

Sze Zheng Yong a,⁎, Marco Gazzino b, Ahmed Ghoniem a

a Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139-4307, USA
b ENEL Ingegneria e Innovazione S.p.A., 56122 Pisa, Via Andrea Pisano 120, Italy

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A steady-state model has been developed to describe the flow and heat transfer characteristics of the slag layer in solid fuel gasification and combustion. The model incorporates a number of sub-models including one for particle capture, and takes into consideration the temperature and composition dependent properties of slag, the contribution of momentum of captured particles and the possibility of slag resolidification. An equally important issue is the interaction of the particles colliding with the slag layer. High inertia particles tend to rebound whereas slower particles are trapped in the slag layer. Since only trapped particles are relevant to the slag layer build-up, a particle capture criterion for colliding particles is introduced. The model predicts the local thickness of the molten and the solid slag layers, the average slag velocity, the temperature distribution across the layer and the heat flux to the coolant, taking into account the influence of molten and resolidified slag layers coating the combustor or reactor wall.

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1. Introduction

Solid fuels and in particular, coal contain inorganic mineral matter. When burned, the inorganic compounds form an incrustable ash residue. In most coal boilers and reactors, coal ash is captured from the flue gas chimneys in the form of fly ash or removed from the combustor bottom as bottom ash. When operating the combustor above the ash fusion temperature, coal ash melts. Some of these molten particles are deposited along the wall, forming a slag layer that flows along the internal walls of the combustion chamber. This molten slag is collected from a molten ash port located at the downstream end of the combustor. The layer of molten slag can act as a thermal barrier to protect the combustor walls. However, because of wall cooling, a portion of this molten slag may resolidify, clogging the molten ash port. Therefore, to maintain a free passage at the molten ash port, understanding the behavior of slag is an integral part of reactor design process.

Several models have been proposed to predict slag formation and its flow characteristics in entrained-flow gasifiers. Seggiani [1] has proposed an analytical time-dependent slag accumulation and flow model to predict both the solid and molten slag layer thicknesses for the gasifier of the IGCC plant in Puertollano, Spain. As an extension to that model, Bockelie et al. [2] introduced a numerical scheme for predicting the molten slag layer thickness. Similarities in both models include the assumptions of negligible shear stress at the slag surface and a linear temperature profiles across both the solid and molten slag layers. Wang et al. [3] used an approach similar to that of Seggiani [1] but included an important feature, that is, the influence of particle deposition on the slag flow momentum. However, Wang et al.’s work stopped short of applying energy conservation to predict the slag temperature, and hence could not predict resolidification.

Suggestions have also been made that particles may more readily captured by a reactor wall that is covered by molten slag layer than in the case of uncovered walls. A model that is able to predict the probability of capture but does not differentiate between particles of different sizes and velocities was given in Shimizu and Tominaga [4]. Benyon [5] has earlier asserted that a crude check of the capture criterion be made based on the angle and velocity of the particle impact. Alternatively, Tominaga et al. [6] suggested that the criterion be based on the viscosities of the slag and incoming particles at the time of collision. Montagnaro and Salatino [7] has confirmed using order of magnitude estimates that the plunging and overlaying of particles are not likely to occur but did not provide a conclusive capture criterion. In contrast, Emory and Berg [8] brought up the role of a vapor film between the particle and slag layer which introduced another element of complication. A simple but more encompassing capture criterion is necessary.

In this paper, we combine the models described in Seggiani [1] and Wang et al. [3]. Moreover, an energy balance is derived for the steady-state case, and a cubic temperature profile across the molten slag layer is used to replace the linear temperature profile assumed in Seggiani [1]. A slag capture criterion is proposed in Section 2.2. The criterion involves determining the stickiness of the slag layer and the impacting particles. This sub-model
deterministically predicts the particles that are captured, as opposed to the probabilistic sub-model used in Wang et al. [3] which was based on Shimizu and Tominaga [6].

2. Slag model

The slag model is developed to better predict the wall boundary condition of a CFD framework for modeling coal combustion or gasification (see Fig. 2). The combustor or gasifier simulation supplies the slag model inputs: the local per unit area particle feeding flux $m_{00}f$, the particle temperature $T_p$, the particle velocity in the direction of slag flow $u_p$, the slag density $q_p$ and the per unit area heat flux to the slag surface $q_{in}$. The slag model computes the slag surface temperature, $T_s$, that is fed back as the wall boundary condition for the next CFD iteration, as well as the average slag velocity, $u_{avg}$, the molten and solid slag thickness, $d_{ml}$ and $d_{sl}$, the inner and the outer wall temperatures, $T_{wi}$ and $T_{wo}$, the mass flow rate per unit length, $m_{00}^e$, and the per unit area heat flux to the coolant, $q_{loss}$. For the slag model, the wall properties and the wall cooling conditions must be supplied and these inputs include the wall thermal conductivity $k_{wall}$, the wall thickness $d_{wall}$, the convective heat transfer coefficient to the coolant $h_{conv}$, the heat loss to coolant $q_{loss}$, the reactor inclination from the horizontal $\alpha$, the total wall thickness $d_{wall}$, the molten slag thickness $d_{ml}$, the solid slag thickness $d_{sl}$, the wall thickness $\delta_{wall}$, the cell slag surface length $\Delta l$, the slag viscosity $\mu_s$, the particle density $\rho_p$, the slag particle surface tension $\sigma_p$, the particle-air surface tension $\sigma_p$, the average shear stress on slag surface $\tau_p$, and the contact angle $\theta$.

2.1. Slag flow model

The slag flow model is based on mass, energy and momentum conservation using the following assumptions:
1. The slag thickness is very small compared to the reactor diameter \((\delta_l + \delta_{slag} \ll D)\).

2. The slag flow is unidirectional, i.e. no reverse flow or flow inhibition is allowed.

3. The shear stress on slag surface, \(\tau_s\), is dominated by the particles captured by the slag layer.

4. The transition temperature between the resolidified and molten slag layers is the slag temperature at the critical viscosity, \(T_{cr}\), which is dependent on the type of coal used as a feedstock.

5. The temperature profile across the molten slag layer is cubic with the following boundary conditions:

\[
T = T_s; \quad \frac{\partial T}{\partial z} = 0, \quad z = 0
\]

\[
T = T_{cr}; \quad \frac{\partial^2 T}{\partial z^2} = 0, \quad z = \delta_l + \delta_{slag}
\]

where \(k\) is the slag thermal conductivity and \(z\) is the distance from slag surface. The cubic profile is chosen based on the von Karman profile method employed in Mills [9] for thin boundary layers with four boundary conditions. This cubic temperature profile is an improvement to previous assumptions of a linear profile by Seggiani [1] and Bockelie et al. [2], as this profile is consistent with the profile observed in the numerical simulation results of Ni et al. [10]. The temperature profile across the molten slag layer is thus given by:

\[
T = T_{cr} + \left(1.5(T_s - T_{cr}) - \frac{m_{in} \delta_l}{2k}\right) \left(1 - \frac{z}{\delta_l}\right)
\]

\[-\left(0.5(T_s - T_{cr}) - \frac{m_{in} \delta_l}{2k}\right) \left(1 - \frac{z}{\delta_l}\right)\] (1)

6. Slag properties are evaluated at the slag mean temperature.

2.1.1. Mass conservation

Fig. 3i illustrates the mass balance for a computational cell \(j\) within the molten slag layer. We assume steady-state in which the mass accumulation rate is zero. Hence, particle deposition rate per unit area \(m_{in}^p\), particle consumption and devolatilization rate per unit volume \(m_{in}^p\) and exit mass flow rate per unit length \(m_{ex}^p\) are related as follows:

\[
\dot{m}_{ex,j} = \Delta \dot{n} + \dot{m}_{ex,j-1} - \dot{m}_{ex,j}^p \Delta x - \dot{m}_{in}^p \delta \Delta x + \dot{m}_{ex,j-1}^p
\]

\[
= \sum_{k=0}^{j-1} \left( \dot{m}_{ex,j}^p - \dot{m}_{in}^p \delta \Delta x / C_0 \right)
\] (2)

where \(j\) is the current computational cell index and \(\Delta x\) is the slag surface length.

The exit mass flow rate per unit length for each cell is given by the average slag velocity \(u_{avg}\) and molten slag thickness \(\delta_l\):

\[
\dot{m}_{ex,j} = \frac{m_{ex}^p}{\pi D} = \rho_s \int_{0}^{\delta_l} u_s(z) \, dz = \rho_s \delta_l \dot{u}_{avg,j}
\] (3)

where \(D\) is the combustor diameter and \(\rho_s\) is the slag density.

As shown in the figure, the particle deposition rate \(m_{in}^p\) is computed from the particle-feed rate \(m_{in}^p\) by subtracting the particle rebound rate \(m_{b}^p\):

\[
m_{in}^p = m_{ex}^p - m_{b}^p
\] (4)

2.1.2. Momentum conservation

Given assumption 1 in Section 2.1, the momentum equation can be expressed in linear coordinates. Furthermore, in the thin layer inertia-free limit, the momentum balance equation can be written as:

\[
\frac{d}{dz} \left( \mu_s \frac{du_s}{dz} \right) = -\rho_g \sin \alpha \quad \text{with} \quad z = 0 \quad \mu_s \frac{du_s}{dz} = -\tau_p; \quad u = 0
\] (5)

where \(\tau_p\) is the average shear stress on the slag surface induced by depositing particles.

Based on Wang et al. [3] and using Eqs. (2) and (3), this average shear stress can be computed as:

\[
\tau_p = \frac{u_{avg}^2 \dot{m}_{in}^p \rho_s \delta_l}{2 \sum_{j=0}^{j-1} (\dot{m}_{ex,j}^p - \dot{m}_{in}^p \delta \Delta x)}
\] (6)

Applying assumption 6 and Eq. (6), the solution of Eq. (5) gives:

\[
\dot{u}(z) = -\frac{\rho_s g \delta_l^2 \sin \alpha}{2 \mu_s} \left(1 - \frac{z}{\delta_l}\right)^2 + \left(\tau_0 \delta_l + \frac{\rho_s g \delta_l \cos \beta}{2 \mu_s}\right) \left(1 - \frac{z}{\delta_l}\right)
\] (7)

Combining Eqs. (2)–(7), the molten slag thickness \(\delta_l\) and the average slag velocity \(u_{avg}\) can be expressed as follows:

\[
\delta_l = \left( \frac{\dot{m}_{ex,j}}{M_p + G_S} \right)^{1/2} = \left( \sum_{j=0}^{j-1} (\dot{m}_{ex,j}^p - \dot{m}_{in}^p \delta \Delta x) / M_p + G_S \right)^{1/2}
\] (8)

\[
u_{avg} = \left( \sum_{j=0}^{j-1} (\dot{m}_{ex,j}^p - \dot{m}_{in}^p \delta \Delta x) \right)^{1/2} (M_p + G_S)^{1/2} / \rho_s
\] (9)

where \(M_p\) and \(G_S\) are defined as:

\[
M_p = \frac{\rho_s u_{avg}^2 \dot{m}_{in}^p}{4 \mu_s \sum_{j=0}^{j-1} (\dot{m}_{ex,j}^p - \dot{m}_{in}^p \delta \Delta x)}
\] (10)

\[
G_S = \frac{\rho_s g \sin \alpha}{3 \mu_s}
\] (11)

2.1.3. Energy conservation

Similar to mass conservation, energy conservation for the molten slag layer for a particular computational cell \(j\) at steady state (see Fig. 3ii) is given by:

\[
\dot{Q}_{ex,j} = \dot{Q}_{in,j} - \dot{Q}_{ex,j-1}
\]

\[
= q_{in} \Delta x - q_{mol} \Delta x - \dot{m}_{in}^p h_{mol} \Delta x + \dot{m}_{ex,j}^p \rho_s \delta_l \Delta x
\] (12)
where $Q_m$ is the exit heat transfer rate per unit length, $m_{mol}$, the melting mass rate per unit area, $h_{mol}$, the heat of fusion, $c_{pp}$, the slag specific heat and $T_p$ the depositing particle temperature.

Employing the proposed cubic temperature profile across the molten slag layer, the exit heat transfer rate per unit length for each cell, $Q_{ex}$, can also be obtained by the following integration:

$$Q_{ex} = g_{ij}c_p\rho_j \int u_j(z)T(z)dz$$

$$= \rho_j c_p \rho_j \frac{q_{ex} \delta_{ij}}{2k_j} \left[ \frac{11 \rho_j g \sin \alpha}{120} + \frac{4 \mu_j M_p j}{15 \rho_j} \right] + T_j \left( \frac{61 \rho_j g \sin \alpha}{240} + \frac{4 \mu_j M_p j}{5 \rho_j} \right) + T_{int} \left( \frac{19 \rho_j g \sin \alpha}{240} + \frac{\mu_j M_p j}{5 \rho_j} \right)$$

(13)

where $M_p$ is given by Eq. (10) and $T_{int}$ is the interface temperature which varies depending on the existence of a solid slag layer. The interface temperature is defined as:

$$T_{int} = \begin{cases} T_{wall} & \text{for } T_{wall} \geq T_{c} \& \delta_{stic} = 0 \\ T_{c} & \text{for } T_{wall} < T_{c} \& \delta_{stic} \neq 0 \end{cases}$$

(14)

where $T_c$ is the temperature at the critical viscosity as defined in assumption 4 and $T_{wall}$ is the internal wall temperature (see Fig. 1). In this derivation, axial conduction has been neglected. This assumption is warranted upon inspection of the Péclet number which is found to be in the order of 1000.

Axial heat conduction is also neglected along the solid slag layer and reactor wall. Thus, the heat flux to the coolant is the heat loss from the molten slag layer $q_{loss}$ yielding the following equations:

$$q_{loss} = \frac{k_{wall}}{\delta_{stic}} (T_{c} - T_{wall}) = \frac{k_{wall}}{\delta_{wall}} (T_{wall} - T_{wall}) = h_s(T_{wall} - T_{c})$$

(15)

where $k_{wall}$ is the solid slag thermal conductivity.

Solving Eqs. (12)-(15) simultaneously and setting the value of $Q_{ex}$ to zero, the unknowns $Q_{ex}$, $q_{loss}$, $T_s$, $T_{wall}$, $T_{co}$ and $\delta_{stic}$ can be computed for each computational cell.

2.2. Particle capture sub-model

The objective of this sub-model is to derive a deterministic capture criterion to predict which particle is captured and which is rebounded. Using this criterion, the mass deposition rate that is needed in Section 2.1 can be determined by using Eq. (4). Capture is defined to include both particles trapped on the surface as well as within the slag layer. Order of magnitude estimates by Montagnaro and Salatino [7] have shown that particles do not penetrate the slag surface unless:

$$d_p V_p > \frac{36H_p}{\rho_p}$$

(16)

where $\rho_p$ is the particle density, $V_p$ the normal component of particle velocity, $d_p$ the particle diameter and $H_p$ the particle viscosity. Since under typical operation conditions, Eq. (16) is not satisfied and a criterion for particle capture on the slag surface is sufficient.

The particle capture criterion is based on the stickiness of the particle and the combustor wall. The particle or the wall is sticky when the particle or the wall temperature is above the ash temperature of critical viscosity [11] and the particle conversion is above a critical particle conversion [12]. Both the temperature of critical viscosity and the critical particle conversion can be determined experimentally. In this work, the critical particle conversion is chosen to be 0.88, in accordance with the experimental results of Li et al. [12].

The Weber number of the impacting particle, which represents the ratio between the kinetic energy and the interfacial surface tension energy between the particle and the slag surface, also plays a role in determining capture. The Weber number is given by:

$$We = \frac{\text{particle kinetic energy}}{\text{surface tension energy}} = \frac{\rho_p V_p^2 d_p}{\sigma_{sp}}$$

(17)

where $\sigma_{sp}$ is the surface tension of the particle if only the particle is molten or of the wall, if the wall is wet. The surface tension is not defined when both the particles are solid and the wall is dry, while for a molten particle impacting a wet wall, the interfacial surface tension, $\sigma_{sp}$, is determined using the Young’s equation:

$$\sigma_{sp} = \sigma_p - \sigma_s \cos \theta$$

(18)

where the contact angle $\theta$ is experimentally determined by Shannon et al. [13] to be $120^\circ$. A particle is rebounded when its Weber number exceeds a critical value. This critical value has been set to 1.

Therefore, depending on the stickiness and the Weber number of the particles, the criteria for particle capture are chosen on the following basis (see Table 1):

1. Experiments have shown that when both the particle and the slag are in the liquid phase (both particle and wall are sticky), the particle is always captured (for all Weber numbers) [14].
2. When dealing with solid–solid interaction, it is assumed that all particles are rebounded.
3. For the case in which the particle is sticky and the wall is non-sticky (dry wall), or when the wall is sticky and the particle is non-sticky, the Weber number criterion is important. Experimental data in Senda et al. [15] indicates the validity of the use of Weber number to differentiate between sticking, reflecting and wall jetting for a liquid droplet on a solid wall. The use of the Weber number criterion is assumed to be also true for the inverse case of solid (non-sticky) particle impacting a liquid (sticky) surface. It is also noted that the range of Weber number of interest excludes the possibility of wall jetting.

3. Simulation results

The slag model is tested under oxy-combustion conditions with inputs from a CFD simulation of an inclined pilot-scale slagging combustor operating at 4 bar. The description of the combustion

![Fig. 4. Combustor geometry (not to scale).](image)
The system is reported in [16,17]. The combustor design is patented by ITEA [18–21]. The combustor geometry is given in Fig. 4. The external wall surface is cooled by water at a temperature of 318 K with an assumed effective heat transfer coefficient of 5.1 W/m² K. Coal water slurry (CWS) with a Sauter mean diameter of 200 µm and coal particle properties given in Table 2 is fed from the top of the reactor.

Fig. 5 shows the CFD simulation outputs which are used as inputs to the slag model, with the exceptions of $q_{\text{loss}}$ and $m_{p0}$, which are model outputs [22]. The heat flux to the slag layer, $q_{\text{in}}$, which is a function of slag temperature, reactor temperature and flow characteristics within the combustor, is obtained from the CFD simulations as the sum of convective and radiative heat fluxes.

The particle feed rate is high at locations without particle capture because of reflected particles that collide with the combustor wall again (Fig. 5b). On the other hand, the particle spray angle adopted in the CFD simulations leads to the low particle temperature at about 0.45 L, as shown in Fig. 5c. The particles that collide with this section of the wall come directly from the atomizer and their residence times are relatively small. While water has been completely evaporated, the particles are still devolatilizing resulting in the low particle temperatures and correspondingly, the largest particle diameter and density because of particle swelling (particle swell ratio is fixed at 1.4). The particles at the two extremes of the combustor wall are fully converted and this can be seen in the plot of particle densities. Note that ash particles are less dense compared to coal particles.

The velocity profiles depend on the flow configuration in the combustor as shown in Chen et al. [22] and reverse flow is observed in the region between 0.2 L and 0.4 L from the combustor inlet. The recirculating flow established at the sudden expansion carries smaller particles with lower inertia back towards the inlet section of the combustor resulting in smaller particle diameters at that section. The gas temperature near the wall, $T_{\text{gas}}$, is lower at the combustor inlet section because of the mixing with fresh oxygen and flue gases while the second half of the combustor, near the exit section is hotter due to the combustion reactions. The results of the slag model presented in the following section are based on steady-state outputs from the CFD. A two-way coupling with the CFD, which will be presented in later publications, is not expected to drastically change the trends observed here.

Table 2 Properties of raw coal and ash.

<table>
<thead>
<tr>
<th>Coal Proximate Analysis</th>
<th>Oxide wt% of ash</th>
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</thead>
<tbody>
<tr>
<td>Moisture (%)</td>
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<tr>
<td>Ash (%)</td>
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<tr>
<td>Volatile matter (%)</td>
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<td>Fixed carbon (%)</td>
<td>43.5</td>
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<tr>
<td>Coal Ultimate Analysis</td>
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<tr>
<td>Na₂O</td>
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<tr>
<td>K₂O</td>
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<tr>
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<td>Cl</td>
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<tr>
<td>Fluorine (ppm)</td>
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</table>

Fig. 5. CFD simulation outputs/model inputs, (a) heat flux to slag surface and heat loss to coolant; (b) mass feed rate per unit area, mass deposition rate per unit area and particle volumetric consumption rate; (c) average particle temperature and gas temperature near the wall; (d) average particle velocity in the direction of and normal to the slag flow; (e) average particle diameter along the wall; (f) average particle density along the wall.
the heat of fusion in Eq. (12) is neglected in this simulation because of the relatively small contribution when compared to the enthalpy of the trapped particles.

3.1. Slag flow model

Flow and heat transfer characteristics of the slag layers are discussed in detail in this section. Slag mass flow rate and velocity apply only to the molten slag layer whereas the slag viscosity is evaluated at the mean temperature of the molten slag layer if it exists. Otherwise, it is evaluated at the surface temperature. The surface temperature $T_s$ and the outer and inner wall temperatures $T_{wout}$ and $T_{win}$ refer to temperatures depicted in Fig. 1. Likewise, heat loss and heat in correspond to $q_{loss}$ and $q_{in}$ as shown in Fig. 3iii.

Fig. 6a shows no slag layer build-up up to approximately 0.4 L from the combustor inlet. This is because of the low temperatures of the walls near the combustor inlet section as can be seen in Fig. 6b. The inner and outer wall temperatures are correspondingly lower than the slag surface temperature because of the finite conductivity through the slag layer and the combustor wall. Note that the trapped particles are on average at a higher temperature than the colliding particles as shown in Fig. 5c. This is the consequence of the critical conversion criterion of the particle capture sub-model. Particles with a higher conversion have higher temperatures due to the combustion process.

No solid slag layer build-up is observed on the combustor wall because of the high temperatures that is common of oxy-combustion environment. The inner wall temperature $T_{win}$ never drops below the temperature of the critical viscosity $T_{cv}$ resulting in no solid slag layer. This is consistent with the definition of solid and molten transition of coal slag at this temperature. This is also coherent with the numerical simulation results of Ni et al. [10] for a coal water slurry gasifier with a refractory wall.

The slag mass flow rate that is observed in Fig. 6c increases steadily down the combustor wall, as more and more particles are captured (see $m_z^n$ in Fig. 5b). On the other hand, the slag velocity increases with increasing particle momentum transfer. The peak velocity is due to the high momentum of the particles that are captured at that location. The momentum of captured particles is dependent on the velocity of those particles in the direction of slag flow, $u_p$. Fig. 5d shows a peak in $u_p$ at that location which once again explains the slag velocity peak. This also accounts for the slight dip in molten slag thickness in Fig. 6a approximately 0.5 L down the reactor. Note that the slag velocity depicted in Fig. 6c is an average across the velocity profile of the molten slag layer in the z-direction obtained from Eq. (5).

The heat loss $q_{loss}$ profile (Fig. 5a) is similar to that of the outer wall temperature $T_{wout}$ (Fig. 6b). Since these two variables can be measured externally, they are good candidates for an overall model validation. Similarly, the slag mass flow rate and the slag viscosity at the molten ash port could be used for model verification.

3.2. Sensitivity analysis

3.2.1. Particle momentum vs. gravity

To study the importance of particle momentum contributions to the slag flow, simulations with various combustor inclinations were performed. Results of these simulations are presented in Fig. 7 where the relative contribution of particle momentum and gravity to slag flow is shown. The same input is used in all the simulations since it is expected to depend on the combustor angle with the horizontal. A peak in particle momentum contribution is observed at approximately 0.4 L down the combustor wall, consistent with the high velocity of the particles that hit that portion of the combustor wall, as shown in Fig. 5d.

Fig. 7a(ii)–c(ii) shows the contribution of particle momentum to the slag thickness. Particle momentum contribution is important for all combustor inclinations. Nonetheless, the gravity contribution cannot be discounted as Fig. 7a(iii)–c(iii) shows an increase in the slag velocity with increasing combustor inclination which accounts for the decreasing molten slag thickness. The temperature profiles in Fig. 7a(iv)–c(iv) have similar trends. However, the temperature drop across the slag layer increases with increasing slag thickness because of the finite thermal conductivity of the slag. It is also notable that no solid slag layer is observed in these cases because of the high temperatures in the combustor.

Fig. 7d(i)–d(iv) shows the case without particle momentum transfer for a combustor inclination of 1.5°. Because of the lower average slag velocity along the combustor wall, the total slag thickness is observed to be thicker and consequently, the temperature difference between the slag surface and the inner wall is significantly larger.

3.2.2. Particle capture sub-model

We next study the influence of the critical Weber number $We_c$ on the slag model. Fig. 8a(i)–c(i) shows the change in mass

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**Fig. 6.** Model outputs, (a) total slag thickness and solid slag thickness, (b) slag surface, inner and outer wall temperatures and temperature at the critical viscosity, (c) slag velocity and mass flow rate, (d) slag viscosity (ordinate in logarithmic scale).
deposition rate per unit area \( \dot{m}_c \) for three different critical Weber numbers: 0.1, 1 and 5. The simulation demonstrates an increase in mass deposition with increasing critical Weber number. A larger \( W_{ec} \) denotes a higher tendency for capture. The figures illustrate that no particles are captured in the top portion of the combustor (up to approximately 0.4 L).

When more particles are deposited, the slag layer should logically be thicker. However, the particle momentum transfer also plays an important role in increasing the slag velocity (Fig. 8a(iii)–c(iii)). As a result, the difference in molten slag layer thickness is observed to be only approximately 0.5 mm, with the exception of the location with a solid slag build-up where the inner wall temperature is below the temperature at the critical viscosity. Here, the solid slag layer can be as thick as 2 mm. Note that a solid layer is build-up at the location where the inner wall temperature dips below the temperature of critical viscosity (Fig. 8c(iv)).

3.2.3. Slag properties

Slag properties vary considerably with temperature and chemical compositions. Therefore, models for slag properties were developed on the basis of these independent variables. Slag properties in this work are evaluated at the slag mean temperature (Assumption 6 in Section 2.1). Given the assumption of a cubic temperature profile across the slag layer (Assumption 5), the mean slag temperature is:

\[
T_{slag} = \frac{5T_s}{8} + \frac{3T_{cv}}{8} - \frac{q_{in} \delta_i}{8k} \tag{18}
\]

where \( \delta_i \) is the molten slag thickness, \( T_s \) the slag surface temperature, \( T_{cv} \) the temperature at critical viscosity, \( q_{in} \) the heat flux to the slag surface and \( k \) the slag thermal conductivity.

The correlations for specific heat, thermal conductivity, density and surface tension are taken from Mills and Rhine [23,24], whereas the slag viscosity is based on the Urbain and the Kalmanovitch-Frank models [25]. When applying these different slag viscosity models, the resulting slag thicknesses can vary up to 0.5 mm and the velocities up to 0.05 mm/s. With the exception of slag viscosity, the variation in the slag properties across the molten slag layer is not significant; making the evaluation of slag properties based on the mean temperature across the slag layer a good approximation. To account for the change in the slag viscosity with the depth from the slag surface, one may modify the approximation by Bird et al. [26] by replacing the linear temperature dependence with the cubic temperature dependence:

\[
\mu(x) = \mu(0) \exp \left[ \left( 1 - \left( 1 - \frac{q_{in} \delta_i}{2k(T_s - T_{cv})} \right)^{1 - \frac{1}{3}} \right) + \left( 0.5 - \frac{q_{in} \delta_i}{2k(T_s - T_{cv})} \right) \left( 1 - \frac{1}{x} \right) \right] \tag{19}
\]

where \( \zeta = -\ln \left( \frac{\mu(x)}{\mu(0)} \right) \).
However, the introduction of this dependence results in the loss of a closed-form solution for the slag model, which increases the computation cost, especially when the slag model is integrated with a CFD simulation.

On the other hand, the temperature of critical viscosity is predicted using correlations presented in Vargas et al. [25] and Seggiani [1]. However, the predictions from these correlations differ considerably and are dissimilar to the experimental value of the
temperature of critical viscosity of the coal used in this study. Therefore, the temperature of critical viscosity is varied to study its influence on the overall slag model.

Fig. 9a(i)–c(i) shows the mass deposition rate per unit area $m_d^0$ at three different temperatures of critical viscosity: 1600 K, 1680 K and 1760 K. As the temperature of critical viscosity is decreased, the simulation shows an increase in mass deposition. This increase is because of the increase of particle stickiness, as mentioned in Section 2.2. The rise in mass deposition also leads to the build-up of slag layer at a location that is closer to the combustor top.

The particles captured because of the rise in particle stickiness are mostly particles of higher velocities (see Figs. 5d and 9a(i)–c(i)). The particle momentum transferred to the layer contributes to the increased slag velocity as the temperature of the critical viscosity decreases. However, the increase in slag velocity does not result in a significant reduction in slag thickness. Hence, as the temperature of critical viscosity is decreased, the slag layer becomes thicker and consequently, the wall temperature becomes lower. However, since the temperature of critical viscosity is also lower, the inner wall temperature does not drop below the ash melting temperature and thus, no solid slag layer is formed.

As we can observe from the sensitivity analysis, the accuracy of predicting the temperature of critical viscosity has a big influence on the simulation results. Therefore, correlations of this temperature should be used with caution and preferably validated by experimental data.

4. Conclusion

A steady-state slag model is presented in this paper. Firstly, the flow and heat transfer characteristics of the slag layers are described. The model is capable of predicting local slag thicknesses, average molten slag velocity, heat fluxes and temperature profiles across the reactor walls. Improvements to existing slag models include the cubic temperature profile across the molten slag layer and the study of particle momentum contributions to the slag layer build-up. Particle momentum contribution is shown to be significant.

Next, a particle capture sub-model with a deterministic capture criterion is described. Initially, a stickiness check of the wall and the impacting particles is performed. The particles are considered sticky when the particle temperature is above the ash melting temperature and if the carbon conversion is above a critical value, while the wall is considered sticky if there is a molten slag layer. This gives four different case permutations: (1) non-sticky wall–non-sticky particle, (2) sticky wall–sticky particle and (3) non-sticky wall–sticky particle and (4) non-sticky particle–sticky wall interactions. Various experiments in the literature have shown that all impacting particles in case (1) rebound and in case (2), they are all captured. For cases (3) and (4), the Weber number is used as a capture criterion because it considers particle velocity and trajectory as well as impacting surface conditions. The critical Weber number is set to 1. Further validation for the particle capture model is necessary since this has a big influence on the results obtained. An alternative way of confirmation is to validate the model as a whole with measurable variables such as outer wall temperature and heat losses to the coolant.

This model also takes into consideration the temperature and composition dependent properties of coal slag. These properties are evaluated at mean temperature of the molten slag layer, assuming the cubic temperature profile as aforementioned. The results of a two-way coupling with the CFD will be presented in a subsequent paper.

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