Numerical investigation of slag formation in an entrained-flow gasifier

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Abstract. A CFD mathematical model for an entrained-flow gasifier is constructed – the model of an actual gasifier is rendered in 3D and appropriately meshed. Then, the turbulent gas flow in the gasifier is modeled with the realizable k-ε approach, taking devolatilization, combustion and coal gasification in account. Various such simulations are conducted, obtaining results for different air inlet positions and by tracking particles of varying sizes undergoing devolatilization and gasification. The model identifies potential problematic zones where most particles collide with the gasifier walls, indicating risk regions where ash deposits could most likely form. In conclusion, effects on the formation of an ash layer of air inlet positioning and particle size allowed in the main gasifier tank are discussed, and viable solutions such as radial inlet positioning for decreasing the amount of undesirable deposits are proposed. We also conclude that the particular chemical reactions that take place inside the gasifier play a significant role in determining how slagging occurs inside a gasifier.

1. Introduction
Although biomass gasification is a well known process, producers of gasifier equipment still face certain problems. Ash melting and deposition phenomena are important problems which cause the formation of a slag layer on equipment walls and may lead to a reliability problem due to negative effects on wall heat transfer and chemical corrosion [1]. Furthermore, slagging is an important phenomenon, but insufficiently investigated both experimentally and numerically. A number of papers describe underlying processes, but linking between local variables of slag (e.g. slag thickness, slag growth speed, slag movement under gravity forces etc.) and global variables of the gas flow is still missing. Most modeling attempts are limited to one or two-dimensional models [2], thus missing spatial behavior of slagging process. This paper aims to explain 3-D effects of particle size and flow characteristics on the formation of slag on the walls of an entrained-flow gasifier.

2. Description of the model
2.1. Geometry
The mathematical model is built on an existing, approximately eight meters high industrial entrained flow gasifier, with dimensions, inlet pipe positions and inlet parameters taken from the technical specification of the gasifier. The gasification process is modeled in 3D. There are two types of geometries being analyzed – the whole gasifier in its entire height, and only the region where the inlet pipes enter the gasifier. This is done to analyze the inlet zone more in detail, as slagging occurs most intensely in that region.
Additionally, to determine how inlet pipe positioning affects slagging tendencies, a few variations of the real inlet zone geometry are constructed, with inlet pipes at various angles, as well as a tilted variant. The different 3D models can be seen in Figure 1. For all cases, in units of bottom inlet diameter (i.e., the diameter of the tank at the bottom is 1), the total height is 2.09, the secondary inlet pipe diameters are 0.065, the inlet pipes connect to the main gasifier tank at a height of 0.83. The top section has a diameter of 1.94 units. The tank begins to widen at a height of 1.11.

![Figure 1. Gasifier geometries with different inlet pipe positioning.](image)

It should be noted that the geometry constructed is only valid for entrained-flow gasifiers—other types of gasifiers, such as the updraft or fluidized bed variants, are built differently, and therefore the results obtained in this paper would not pertain to gasifiers that differ strongly in principle from entrained-flow gasifiers. The results are valid only as long as the oxidizing agent and the biomass are fed co-currently through the gasifier, though, as we note later, the particular geometry and chemical reactions taking place are important to the result, even if the gasifier type matches with the one considered in this paper.

2.2. Gas mixture and flow
The gas inside the gasifier is modelled as an incompressible ideal gas. The flow regime of the gas mixture inside the gasifier is turbulent, and the realizable $k$-$\varepsilon$ turbulence model is used to account for such behaviour in the model. In the $k$-$\varepsilon$ model, two governing equations are solved—the turbulent energy equation (for $k$) and the turbulent dissipation equation (for $\varepsilon$) in addition to the Navier-Stokes equation. Furthermore, heat transport is also modeled via the energy transport equation. The equations are solved numerically in ANSYS Fluent software in a mesh consisting of approximately 800k elements, with the number slightly varying over different geometries.

At the bottom of both models, a gas mixture ($CO - 45\%$, $N_2 - 26\%$, $CO_2 - 16\%$, $H_2O - 6\%$, $CH_4 - 6\%$, $H_2 - 1\%$) at 873 °C temperature is introduced at a constant mass flow rate consistent with operating conditions. The composition of this mixture was obtained from a separate calculation. There is a stage the biomass undergoes before entering the gasification chamber—first, it experiences a stage of devolatilization. This process was calculated separately, and the resultant gas mixture was then applied to the main model. This gas flow drives the co-current flow of the gasifier. Additionally, from every side inlet, a mixture of air and steam is introduced at 1073 °C, also at a constant mass flow rate. The mixing of these two flow sources and the resultant velocity field determines the behavior of particles as they travel through the gasifier.

As thermal effects are important for the process of gasification, the energy equation is also enabled. Thus, heat transfer due to diffusion, species transfer, chemical reactions etc. are taken in account. The heat flux through the gasifier walls is assumed to be zero.

2.3. Particles and gasification
Particles are introduced into the gasifier via the bottom at a constant mass flow rate. To investigate the role of particle sizing in slagging tendencies, four particle sizes were chosen—5 µm, 100 µm, 500 µm, and 1 mm in diameter. The particles are made up of 80% coal and non-combustibles. The process of
devolatilization takes place before the particles enter the gasifier, so volatile fraction is low. For all simulations, the mass flow rate of each type of particle is the same.

Because there are no more than a few hundred thousand particles inside the transition zone at any time, the particles constitute a very small volume fraction (no more than 0.05%) and thus the particle trajectories can be modelled using the Lagrangian approach.

The forces governing particle trajectory are as follows: inertial forces, gravity (facing downwards in the geometry sketches), thermophoretic force and a turbulence random walk force (with the characteristic time scale taken 0.30k/ε). The thermophoretic force manifests itself for particles smaller than a millimeter and is of the form:

\[ \vec{F} = -D \frac{1}{mT} \nabla T \]

Here, \( D \) is the thermophoretic constant, \( m \) is the mass of the particle, \( T \) is the temperature around the particle, and \( \nabla T \) is the gradient of the temperature.

The dominant forces in trajectory determination are the forces of inertia and gravity. The thermophoretic force adds small corrections, and the turbulence random walk model is enabled to account for small fluctuations of the turbulent gas flow that disappear when doing numerical calculations over averaged time steps – it adds a component of velocity to the mean velocity with a set of randomly generated normally distributed variables:

\[ u_i' = \zeta_i \sqrt{\frac{u_i^2}{u_i}} \]

Here, \( u_i \) is the i-th component of the fluctuation velocity, \( \zeta \) is the random variable for that component of velocity, and the remaining term is the RMS of the i-th velocity component. The random variables are generated anew every time the fluctuations are applied (which is over a period equal to the time scale mentioned previously).

While the particles make their way through the gasifier, they also undergo chemical reactions that produce syngas. Additionally, there are reactions that take place in the volume of the gas as well. All reaction rates are modelled with the Arrhenius equation. The reactions taken in account are summarized in Table 1.

| Reaction type | Reaction equation | A       | E, J/kmol | Reference |
|---------------|-------------------|---------|-----------|-----------|
| Volumetric    | CO + 0.5O\(_2\) → CO\(_2\) | 2.239×10\(^{12}\) | 1.67×10\(^{6}\) | [3]       |
| Volumetric    | CO + H\(_2\)O → CO\(_2\) + H\(_2\) | 9.87×10\(^{8}\) | 3.1×10\(^{7}\) | [4]       |
| Volumetric    | CO + 3H\(_2\) → CH\(_4\) + H\(_2\)O | 5.12×10\(^{14}\) | 2.73×10\(^{4}\) | [3]       |
| Volumetric    | H\(_2\) + CO\(_2\) → CO + H\(_2\)O | 1.785×10\(^{12}\) | 3.26×10\(^{8}\) |           |
| Volumetric    | CH\(_4\) + 1.5 O\(_2\) → CO + 2H\(_2\)O | 5.012×10\(^{11}\) | 2×10\(^{8}\) | [5]       |
| Volumetric    | CH\(_4\) + H\(_2\)O → CO + 3H\(_2\) | 5.922×10\(^{8}\) | 2.09×10\(^{6}\) | [6]       |
| Surface       | C\(\_s\) + 0.5O\(_2\) → CO | 300     | 1.3×10\(^{8}\) | [7]       |
| Surface       | C\(\_s\) + CO\(_2\) → 2CO | 2224    | 2.2×10\(^{8}\) | [7]       |
| Surface       | C\(\_s\) + H\(_2\)O → CO + H\(_2\) | 42.5    | 1.42×10\(^{8}\) | [7]       |
| Surface       | C\(\_s\) + 2H\(_2\) → CH\(_4\) | 1.62    | 1.5×10\(^{8}\) | [7]       |

The particles are decoupled from the flow – first, the flow fields are calculated, then the particles trace through the acquired flow.
3. Results and discussion

3.1. Particle behaviour with no gasification reactions

To first see the isolated effect of the flow inside the gasifier tank on particle collisions with the walls of the gasifier, calculations that omit chemical reactions were made. These calculations were made on all geometry variants to see how inlet positioning can determine critical zones where slag deposition is most intense. The obtained flow velocity fields can be seen in Figure 2.

When the inlets are positioned tangentially with respect to the walls, the flow tends to swirl in the radial direction, but is mostly straight in the axial direction. In this regime, particles experience a centrifugal force as they travel upwards through the gasifier, which plays a role in particle collisions with the walls. When inlets are radial, secondary vortices appear in the axial cross-section. Here, the particles that sediment on the walls are those that are pulled inside these vortices and guided towards the walls.

![Figure 2](image_url)

**Figure 2.** Flow velocity fields for all geometry variations – from above (top) and from the side (bottom). The left side scale is for the first three cases, the right-side scale is for the latter two cases.

Next, particle behaviour in all models was analysed. A simple wall collision model was used – every particle that hit a wall was terminated, and the position and size of the particle was reported. The obtained data is summarized in Table 2 and Figure 3.

| Model (refer to Figure 1) | a    | b    | c    | d    | e    |
|---------------------------|------|------|------|------|------|
| **Total collisions**      | 1450000 | 1591463 | 1776187 | 1953891 | 758868 |
| **Total collisions, normalized** | 1.91 | 2.10 | 2.34 | 2.57 | 1.00 |
| 5 µm, %                   | 5.3  | 9.5  | 10.7 | 2.4  | 2.8  |
| 100 µm, %                 | 26.6 | 35.1 | 35.5 | 13.9 | 11.0 |
| 500 µm, %                 | 47.5 | 39.6 | 36.9 | 47.6 | 38.3 |
| 1 mm, %                   | 20.7 | 15.8 | 16.9 | 36.1 | 47.9 |

Table 2. Results for particle collision in the model with no chemical reactions.
From the simulations, it is evident that the problematic slagging zones become more pronounced as the inlets are made more radial. In particular, a spike in collisions occurring immediately below the inlets arises once the inlets become radial (Figure 3 d and e). It is also notable that for tangential inlets (Fig 3 a and b) the collision zones are broad, owing to the centripetal forces that push transiting particles toward the walls. As the inlets are turned more radially, the broad impact zones tend to become sharper and center around the inlet zones due to secondary vortices that form immediately below the inlets and push particles toward the problematic zone.

Furthermore, larger particles (500 µm and 1 mm) generally tend to collide with the walls at low heights more than the smaller particles. This is especially evident in the tangential inlet configuration (Fig 3. a, b, c). As the heavy particles travel through the gasifier slower than smaller ones, they are exposed to the centrifugal forces for a longer time, allowing for collisions. Conversely, the 100 µm particles collide the least relative to the rest (see Table 2) – this is because the small particles can pass the inlet zone before colliding with the walls at all.

An interesting dynamic occurs when the radial inlets are tilted (Figure 3. e) – the total amount of particles experiencing collisions is the lowest of all possible configurations, however, the collision zone is very pronounced. In other words, there is a potential risk of forming a slag ring. To fully argue whether slagging occurs at the walls, though, gasification reactions must be taken in account and a more sophisticated trapping condition must be formulated for the particles.

![Figure 3. Histogram of amount of particles hitting the walls depending on the height of impact (numeration consistent with Figure 1).](image-url)
3.2. Particle behaviour with no gasification reactions

Next, the full gasification model is enabled, allowing the gas and particles to chemically react with the gases present as described previously. Also, a more adequate trapping condition is formulated, based on the fusion temperature of the particles and conversion rate, which is calculated as follows [10]:

$$X = 1 - \frac{C_{\text{char}} C_{\text{ash}}}{(1 - C_{\text{char}}) C_{\text{coal}}} \quad (3)$$

where $X$ is the conversion rate of the particle and $C$ is the weight fraction of the material in the top index in the bulk of the material in the lower index.

The condition depends on the state of both the particle and the wall [8,9,10]. The particle can be in either a sticky state (its temperature above fusion temperature, particle conversion above critical value) or a non-sticky state. Also, the fate of the particle depends on the Weber number ($We$), which shows the ratio between inertial forces in the fluid and surface tension:

$$We = \frac{\rho v^2 l}{\sigma} \quad (4)$$

Here, $\rho$ is the density of the fluid, $v$ is the velocity of the particle, $l$ is the characteristic length of the particle and $\sigma$ is the surface tension.

There are different scenarios depending on whether the Weber number is above or below a critical value (taken to be 1). Similarly, the wall is deemed sticky if it is above the fusion temperature of the particle or if the impeding particle is sticky. The subsequent scenarios are summarized in Table 3.

| Table 3. Particle slagging conditions [8]. |
|------------------------------------------|
| Sticky particle                          | Non-sticky particle |
| Sticky wall                              | $We$<1 | $We$>1 | $We$<1 | $We$>1 |
|                                        | Slagging | Slagging | Slagging | Reflect |
| Non-sticky wall                          | Slagging | Reflect | Reflect | Reflect |

With these conditions in place, a simulation was run. The flow fields were practically unchanged relative to those depicted in Fig. 2, allowing to conclude that gasification processes do not dramatically change the flow characteristics. However, particle collisions are vastly different. The amount of collisions decreases rapidly in this model, and the tangential models report approximately 100 times more collisions than radial models as shown in Table 4. To explain this, temperature fields of cases a, d and e are shown in Fig. 4.

| Table 4. Results for particle collision in the model with enabled chemical reactions. |
|------------------------------------------|
| Model (refer to Fig. 1)   | a   | b   | c   | d   | e   |
| Total collisions           | 987644 | 996731 | 769458 | 14842 | 10097 |
| Total collisions, normalized | 97.82 | 98.72 | 76.21 | 1.47 | 1 |
| 5 µm, %                   | 5.3 | 9.5 | 10.7 | 2.4 | 2.8 |
| 100 µm, %                 | 26.6 | 35.1 | 35.1 | 13.9 | 11.0 |
| 500 µm, %                 | 47.5 | 39.6 | 36.9 | 47.6 | 38.3 |
| 1 mm, %                   | 20.7 | 15.8 | 16.9 | 36.1 | 47.9 |

For the tangential cases, temperature spikes are located near the walls. In accord with the particle sticking condition, this makes particles prone to slagging. Also, as previously explained, large
particles are mostly forced towards the walls in the tangential configurations due to centripetal forces, further increasing the risk of excessive slag with large particle aggregation. The temperature spikes around the inlets and close to the walls are also reported experimentally, indicating that the model gives results that coincide with reality and giving a certain degree of validation.

Conversely, in the radial cases, the temperature spikes are in the middle, away from the walls. This gives an inverse effect – the gas temperature near the walls is relatively low, predominantly cooling the wall and particles, tending them towards non-sticky scenarios.

![Figure 4. Temperature fields for various models with enabled gasification reactions.](image)

It is important to take into account gasification reactions, as they determine the heat distribution inside the gasifier. As just shown, particle and wall temperature plays a large role in determining whether slag will form, overriding the tendencies appearing just from the analysis of the gas flow with no reactions. Thus, the probability of excessive slag deposition is also dependent on the particular geometry of the gasifier, though it appears that in axially symmetrical cases tangential inlets lead to temperature spikes near walls, significantly increasing the danger of slagging. To avoid slagging, a radial configuration for inlets is recommended.

4. Conclusions

A model for gasification in an entrained-flow gasifier was created and run in two modes – without the gasification chemical processes taking place, and then with the processes taken into account. The first model was used to analyze the impact of the flow inside the gasifier on the particles passing through it. It was determined that tangentially positioned inlets create a swirling flow that gives rise to centripetal forces that push particles towards the walls. Smaller particles experience this less as they travel through the gasifier quickly, but larger particles tend to collide with the walls because of this. In radial inlet configurations, a secondary vortex arises that pushes particles into a zone directly below the inlets.

In the second simulation run, gasification reactions are enabled and a more sophisticated particle capturing condition is formulated. With these in place, a dramatic change is reported – particles collided with walls far more in tangential configurations than radial ones. This is explained by the temperature fields in the gasifiers – in tangential cases, the largest temperatures are near the walls, while for radial cases the heat spikes are located in the middle. Therefore, a tentative recommendation to reduce excessive slagging can be made - slagging is decreased for gasifiers with axial symmetry if the inlets are positioned radially as opposed to a tangential positioning.

Finally, it is determined that chemical reactions inside the gasifier take a predominant role in determining slagging processes and potential risk regions, taking precedence over the flow profile inside the gasifier. Thus, it is important to take chemical processes in account when modelling slagging due to gasification.
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