Proceedings of the
THIRD INTERNATIONAL
SLAG VALORISATION
SYMPOSIUM
THE TRANSITION TO SUSTAINABLE MATERIALS MANAGEMENT

19-20 March 2013
Leuven, Belgium

Editors
Annelies Malfliet, Peter Tom Jones, Koen Binnemans, Özlem Cizer, Jan Fransaer, Pengcheng Yan, Yiannis Pontikes, Muxing Guo, Bart Blanpain
EFFECT OF GAS-SLAG INTERACTION ON VALORISATION OF HIGH TEMPERATURE TREATED WASTE

Pengcheng YAN, Lieven PANDELAERS, Lieven MACHIELS, Yiannis PONTIKES, Muxing GUO, Bart BLANPAIN

Department of Metallurgy and Materials Engineering, KU Leuven, 3001 Heverlee, Belgium
pengcheng.yan@mtm.kuleuven.be; lieven.pandelaers@mtm.kuleuven.be; lieven.machiels@mtm.kuleuven.be; yiannis.pontikes@mtm.kuleuven.be; muxing.guo@mtm.kuleuven.be; bart.blanpain@mtm.kuleuven.be

Abstract

During the high temperature treatment of organic-rich wastes to produce energy, a gasified organic fraction is often in contact with a molten inorganic fraction, i.e. a slag. Depending on the degree of gas-slag interaction, gas and slag compositions may vary and consequently influence the valorisation potential. To evaluate the influence of this interaction, a pseudo-kinetic model was developed based on local thermodynamic equilibrium between the gas phase and part of the slag. The interaction level was accounted for by varying the amount of the slag that equilibrates with the gas. The valorisation potential of the resulting gas and slag phases was evaluated in terms of the heat of combustion and the mineralogy after cooling, respectively. The production of a metal phase was also considered.

Introduction

Waste streams containing high amounts of organic material can be valorised by converting them to an energy-rich syngas. If the treatment temperature is high enough, of the order of 1400°C, a partially or completely molten slag phase, which contains the inorganic waste fraction, is formed as by-product. Ideally, this slag can be valorised after cooling, for instance in construction applications. However, the specific valorisation route and the associated added-value are intimately related to the mineralogy of the slag which in turn depends on the slag composition, as well as the cooling profile. Whereas the cooling profile can be controlled after (and/or during) tapping the slag, the slag composition is highly influenced by the process itself, i.e. the gas-slag interaction in the reactor. This process may become increasingly complex, if a metal phase is formed as a consequence of the gas-slag interaction.

Predictions based on thermodynamic and kinetic modelling are a valuable tool to complement experimental analyses of this gas-slag interaction. One approach is to use only thermodynamic data and to introduce kinetics in a pragmatic way. In the present
Figure 1: Schematic representation of high temperature gas-slag interaction in inorganic waste treatment

paper, an effective equilibrium reaction zone model is used that assumes equilibrium in a reaction zone at the gas/liquid interface \(^2\,^3\) (Figure 1). The kinetics are indirectly accounted for by varying the size of this reaction zone, i.e. the percentage of the gas and slag phases involved in the equilibrium calculation for the considered time step.

The aim of the present paper is to simulate the gas-slag interaction during high temperature treatment based on an effective equilibrium reaction zone (EERZ) model. The influence of the reactive slag fraction, i.e. the percentage of slag involved in the equilibrium calculation, on the valorisation potential of the products, in terms of the heat of combustion for the gas product, the mineralogy of the slag after cooling and the metal formation, was investigated.

**Model setup**

As shown in Figure 1, \(x\) wt% gas and \(y\) wt% slag reacts at their common interface to reach equilibrium at the EERZ. Thereafter, this equilibrated gas is assumed to instantaneously mix with the rest of the bulk gas and flows out of the reactor (off gas). The equilibrated slag also uniformly mixes with the rest of the bulk slag. If the mixing of gas generates additional slag, or vice versa, the mixing routine is iterated until no new slag or gas is generated. To simplify the calculations, it is assumed that the pressure and temperature in the reactor are constant in space and time and set at 1 atm and 1400°C, respectively. Moreover, the metal phase is assumed to sink to the bottom and does not interact with the gas after it has formed. The thermodynamic software FactSage was linked to the custom made model through the Chemapp interface (GTT-Technologies). The FactPS and FToxide databases were used. The initial gas and slag compositions used in the calculation are listed in Tables 1 and 2, respectively. The overall mass ratio of gas/slag was set to 1.1 in the model. Due to the fact that the diffusion is much faster in the gas phase than in the slag phase, it was assumed that all the gas reacted with part of the slag during the treatment, i.e. \(x = 100\).
Table 1: The gas chemistry used in the calculation (wt%)

<table>
<thead>
<tr>
<th>CO</th>
<th>CO₂</th>
<th>H₂</th>
<th>CH₄</th>
<th>N₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>12</td>
<td>17</td>
<td>1</td>
<td>50</td>
</tr>
</tbody>
</table>

Table 2: The slag chemistry used in the calculation (wt%)

<table>
<thead>
<tr>
<th>FeO</th>
<th>Fe₂O₃</th>
<th>SiO₂</th>
<th>CaO</th>
<th>MgO</th>
<th>Al₂O₃</th>
<th>MnO</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.3</td>
<td>34.3</td>
<td>14.1</td>
<td>15.2</td>
<td>2.0</td>
<td>6.1</td>
<td>3.0</td>
</tr>
</tbody>
</table>

Results and discussion

Figures 2 and 3 shows the effects of the reactive slag fraction, i.e. the percentage of slag involved in each iteration of the gas-slag interaction, on the amount and composition of the reaction products, the enthalpy requirement of the reactor, which is the enthalpy difference between the final products and the initial reactants, as well as the mineralogy of the solidified slag.

The amount of produced metal (mainly Fe) increases linearly with the reactive slag fraction (Figure 2a). Practically, this means that more metal is produced as the contact between the gas and the slag is improved, for instance by stirring the slag. The total heat of combustion (room temperature and sufficient oxygen) for the obtained gas decreases with increasing reactive slag fraction, even though the total amount of gas increases (Figure 2b). As a consequence, an increase in the valorisation potential through metal production will be off-set by a decrease in the energy content of the gas.

The metal formation and the changes in the gas composition also affect the slag composition. The FeO to Fe₂O₃ ratio increases with increasing reactive slag fraction (Figure 3a), while the amounts of FeO and Fe₂O₃ are decreasing due to the reduction of FeₓOᵧ to Fe by the gas. The FeO/Fe₂O₃ ratio influences the slag mineralogy after solidification and consequently the valorisation potential. Here, the mineralogy of the obtained slag at room temperature is predicted by assuming equilibrium cooling.

![Figure 2: The influence of the reactive slag fraction on: (a) gas-slag interaction products and (b) gas composition excluding N₂](image-url)
conditions (Figure 3b). Spinel, which can incorporate a number of elements, e.g. Mn, Al and Cr, has considerable influence on the slag valorisation potential\(^4\). For an increasing reactive slag fraction the amount of spinel decreases, showing the effect of high temperature interaction on slag valorisation potential (Figure 3), i.e. the decrease of FeO/Fe\(_2\)O\(_3\) ratio limits the formation of Fe\(_3\)O\(_4\).

Thus, depending on the valorisation focus, this process allows significant flexibility only by controlling the level of interaction between the slag and the gas. Moreover, an optimised reactive slag ratio can be obtained by aiming for an overall maximum valorisation value (depending on the market) from the gas, slag and metal products.

**Conclusion**

The gas-slag interaction in the high temperature treatment of organic-rich wastes was simulated with a pseudo-kinetic model, based on an effective equilibrium reaction zone. The influence of the interaction level on the amount, composition and mineralogy of the reaction products was investigated. It is shown that the amount of metal, the heat of combustion for the produced gas as well as the slag composition and consequently the slag mineralogy after solidification depend strongly on the gas-slag interaction, allowing a large degree of flexibility in the treatment depending on the valorisation focus.

**References**