Development of a modular mathematical model for the EAF process

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Introduction

Aims

• This work aims to develop a model for online prediction of the EAF process.
  - Compositions
  - Temperatures
  - Heat losses
  - Energy efficiency
• The model should be applicable for model predictive control.
• The model should also serve as an offline tool for process development.
Structure of the model

Overview of the modules

1. Heat and mass balance and scrap melting
   - Scrap melting rate
   - Heat content of phases

2. Gas phase reactions in the freeboard
   - offgas composition
   - heat losses to offgas

3. Metal-slag reactions in the flat bath
   - metal composition
   - slag composition
Structure of the model
Scrap melting module

Working principle

- A dynamic model developed in the master’s thesis of Ringel [1].
- Solves the energy and mass balances of the system.
- Serves as the core of the overall model.
- Time integration is conducted using an adaptive 4th Runge-Kutta method.

Reference
Radiative heat transfer: main assumptions

- The electrode has bored into the scrap pile and the molten surface is exposed.
- The furnace is depicted as a cylinder without the step formed by refractory material.
- The three electrodes of AC furnaces are modelled as a single electrode, which forms a cylindrical hole in the scrap.
- Both the top slag and the gap between the electrodes and the roof are neglected.
Structure of the model
Scrap melting module

Radiative heat transfer: view factors

- The radiative heat transfer can be calculated based on view factors and radiosities.

- The radiative heat flux is given by

\[ Q_{i-RAD} = A_i \cdot \sum_{j=1}^{N} VF_{ij} \cdot (J_i - J_j) \]

- The radiosity can be calculated as follows:

\[ J_i = \varepsilon_i \cdot \sigma_{SB} \cdot T_i^4 + (1 - \varepsilon_i) \cdot \sum_{j=1}^{N} (VF_{ij} \cdot J_j) \]

- The view factor \( VF \) is a ratio of the share of radiation from a surface to another surface.

<table>
<thead>
<tr>
<th>number</th>
<th>zone</th>
<th>emissivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>roof</td>
<td>0.85</td>
</tr>
<tr>
<td>2</td>
<td>wall</td>
<td>0.85</td>
</tr>
<tr>
<td>3</td>
<td>solid scrap</td>
<td>0.80</td>
</tr>
<tr>
<td>4</td>
<td>liquid scrap</td>
<td>0.40</td>
</tr>
<tr>
<td>5</td>
<td>arc</td>
<td>1.00</td>
</tr>
<tr>
<td>6</td>
<td>electrode</td>
<td>0.75</td>
</tr>
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</table>

View factor matrix.
Electric arc

- The arc length is calculated using the correlation by Bowman [1] assuming the electrodes are cylindrical and homogeneous with respect to current and temperature.
- The arc resistivity was taken from Jones et al. [2].

References
Burners

- The natural gas injected is assumed to be pure methane (CH\textsubscript{4}).
- The burner efficiency is solved according to a hyperbolic tangent function [1–3].
- The reaction enthalpy is solved using an embedded thermochemistry module.

Reaction enthalpy of the combustion of methane

Burner efficiency as a function of temperature.

References
Structure of the model
Scrap melting module

Thermochemistry
- Based on a previously-developed thermochemistry module for hot metal desulfurization [1].
- Calculates thermochemical data such as:
  - The specific heat capacity of components and mixtures.
  - Enthalpy, entropy and Gibbs energy of individual species, mixtures and reactions.
- Accounts for the following components:

<table>
<thead>
<tr>
<th>Metal</th>
<th>Slag</th>
<th>Gas</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe, C, Si, Cr, Mn, P</td>
<td>FeO, SiO$_2$, Cr$_2$O$_3$, MnO, P$_2$O$_5$, CaO, MgO, Al$_2$O$_3$</td>
<td>N$_2$, O$_2$, CO, CO$_2$, CH$_4$</td>
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</tbody>
</table>

Reference

Specific heat capacity and enthalpy of iron.
Structure of the model
Gas phase reaction module

Working principle

- The gas phase reaction module was developed by Jussila [1].
- In this work, the gas phase reactions were modeled as equilibrium reactions.
  - The Gibbs energy minimization in the freeboard was executed using the Lagrangian steepest descent method by White et al. [2].
  - The approach was coupled with the initial value calculation by Blecic et al. [3].
- The module can be used for any gas-phase equilibrium calculations.

![Diagram of the model's structure]

References

Execution of the steepest descent method.
**Structure of the model**

**Metal–slag reaction module**

**Working principle**

- The metal–slag reaction module by Hekkala [1] describes the kinetics of mass transfer controlled reactions.
- The distribution of oxygen is calculated using the effective equilibrium constant method by Robertson et al. [2].
  - Basically an extension of the two film theory.
  - The equilibrium at the interface is obtained by solving an electronegativity equation for oxygen.
- The activity coefficients for metal and slag components are calculated using the UIP formalism [3] and RSM model [4], respectively.

**Molar flux of species** $M$

\[
J_M = \frac{\beta_L \rho_L}{100M_M} \left( [\%M] - [\%M]^* \right) \quad \text{(in metal)}
\]

\[
= \frac{\beta_S \rho_S}{100M_{MO_x}} \left( [%MO_x]^* - [%MO_x] \right) \quad \text{(in slag)}
\]

**Electronegativity equation at the interface**

\[
\sum_{M=1}^{n} J_M v_{M,O} = 0
\]

**References**

Results and discussion
Scrap melting module

Preliminary results

- The model seems to provide a realistic trajectory for the melting of scrap.
- Quantitative analysis, however, is not possible as the amount of liquid scrap is unknown.

An example on the simulated scrap melting as a function of time.
Results and discussion

Gas reaction module

Verification

- Table shows a comparison of methods for an example case.
- A perfect or near-perfect agreement with the studies by White et al. [2] and Blecic et al. [3].
- Also, a very good agreement with HSC Chemistry.
- The model was later applied for gases relevant for the EAF atmosphere.

<table>
<thead>
<tr>
<th>Species</th>
<th>Study</th>
<th>Error in abundance vs Jussila [1]</th>
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</thead>
<tbody>
<tr>
<td>H</td>
<td>0.040655</td>
<td>0.040668</td>
</tr>
<tr>
<td>H₂</td>
<td>0.147710</td>
<td>0.147730</td>
</tr>
<tr>
<td>H₂O</td>
<td>0.783187</td>
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</tr>
<tr>
<td>N</td>
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</tr>
<tr>
<td>N₂</td>
<td>0.485248</td>
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</tr>
<tr>
<td>NH</td>
<td>0.000693</td>
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<tr>
<td>NO</td>
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<td>0.027399</td>
</tr>
<tr>
<td>O</td>
<td>0.017941</td>
<td>0.017947</td>
</tr>
<tr>
<td>O₂</td>
<td>0.037309</td>
<td>0.037314</td>
</tr>
<tr>
<td>OH</td>
<td>0.096857</td>
<td>0.096872</td>
</tr>
</tbody>
</table>

Virtually no error

Equilibrium abundances for the combustion of hydrazine and oxygen at 3500 K and 750 psi [1].

References

Verification and validation

- Functional validation of the metal-slag reaction module will be finished using the case by Ohguchi et al. [1].
- The overall validation of the model is to be finished with plant data from carbon steelmaking and stainless steelmaking.

OES measurements

- The model is intended to be coupled with OES-based online measurements for detecting deviations from the intended melting "trajectory".
  - When the scrap is molten?
  - What is the composition of the slag?

<table>
<thead>
<tr>
<th>Collaborators</th>
<th>Topics</th>
</tr>
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<tbody>
<tr>
<td>Luxmet Oy</td>
<td>Control systems for EAF</td>
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<td></td>
<td>OES measurements</td>
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<td>RWTH Aachen University</td>
<td>Modelling methodology</td>
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<td>Heat transfer</td>
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<td>Laboratory experiments</td>
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<td>Ovako Imatra Oy</td>
<td>Scrap-based carbon steelmaking</td>
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<td>Outokumpu Stainless Oy</td>
<td>Scrap-based stainless steelmaking</td>
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<td></td>
<td>Alternative EAF technologies</td>
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</table>
Adaptivity

- Tuning parameters are needed to adapt the model to process data.
- In this work, the aim is to apply machine learning for automatic adaptation of the model to process data.
Conclusions

- This work aimed at developing a fundamental mathematical model of the EAF process for online use.
- So far, stand-alone modules have been developed for
  - scrap melting
  - gas-phase reactions in the freeboard
  - metal–slag reactions
- The next steps are to couple the modules together into a single model and validate the model with plant data.
- The use of online OES measurements to support model predictions will also be tested.

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