Development of a modular mathematical model for the EAF process

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Contents

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

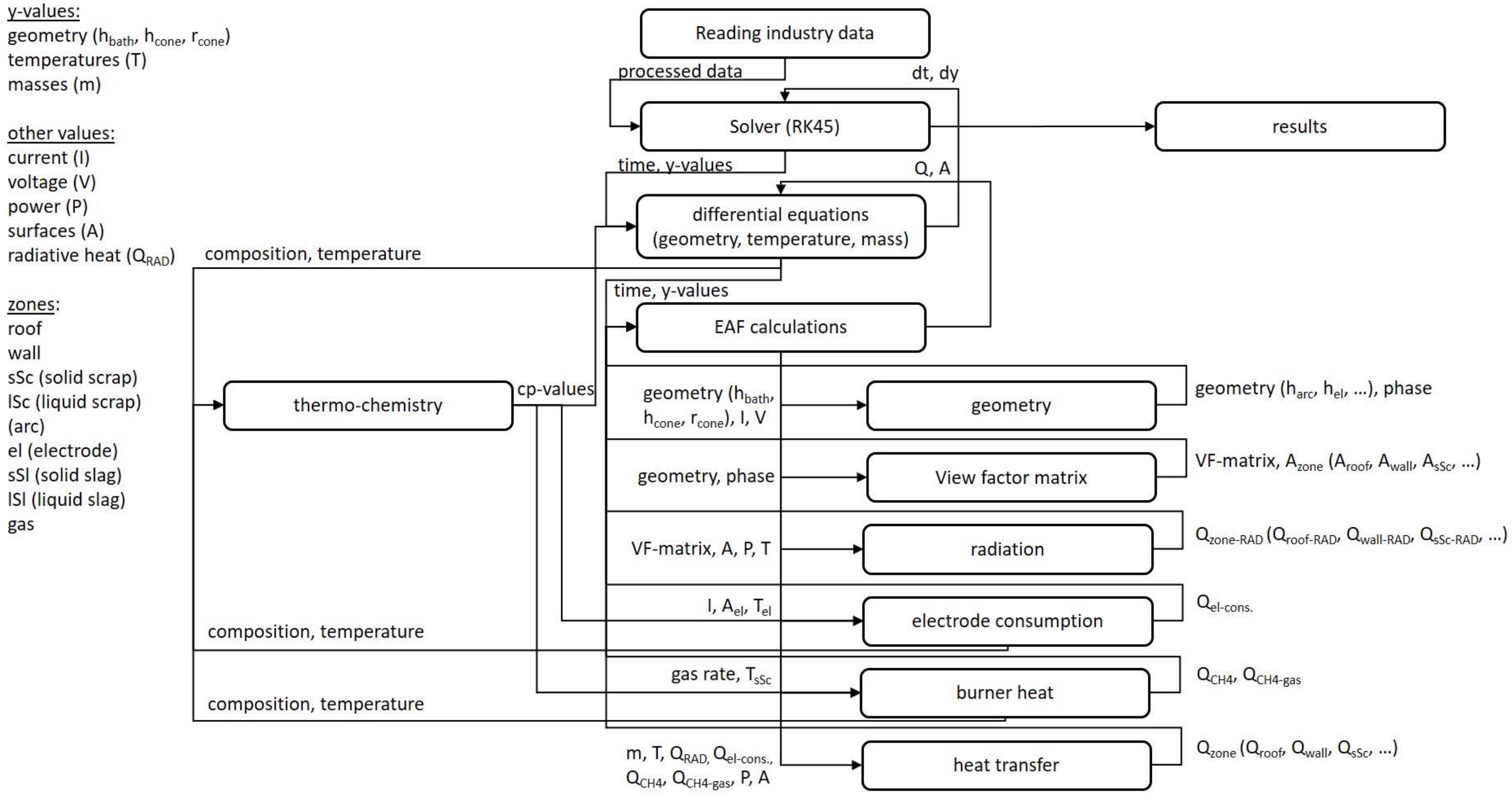
3. Metal-slag reactions in the flat bath
   - ❑ metal composition
   - ❑ slag composition

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.



Schematic illustration of the scrap melting module.
A. Ringel, Master's thesis, RWTH Aachen University, 2020.

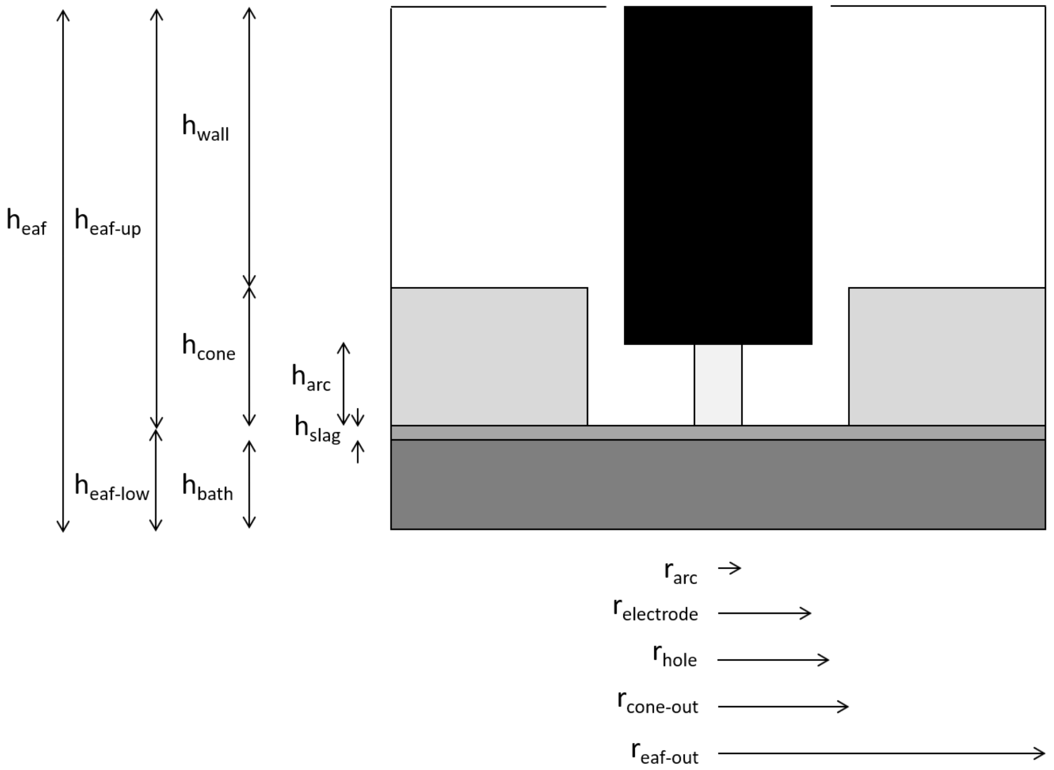
Reference
[1] A. Ringel, Master´s thesis, RWTH Aachen University, 2020.

Structure of the model

Scrap melting module

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.



Geometry of scrap melting.
A. Ringel, Master’s thesis, RWTH Aachen University, 2020.

Structure of the model

Scrap melting module

number	zone	emissivity
1	roof	0.85
2	wall	0.85
3	solid scrap	0.80
4	liquid scrap	0.40
5	arc	1.00
6	electrode	0.75

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

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

- 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 is the share of radiation from a surface to another surface.

from (…) zone \ to (…) zone	roof (1)	wall (2)	sSc (3)	lSc (4)	arc (5)	electrode (6)
roof (1)	0	VF_{1-2}	VF_{1-3}	VF_{1-4}	VF_{1-5}	VF_{1-6}
wall (2)	VF_{2-1}	VF_{2-2}	VF_{2-3}	VF_{2-4}	VF_{2-5}	VF_{2-6}
sSc (3)	VF_{3-1}	VF_{3-2}	VF_{3-3}	VF_{3-4}	VF_{3-5}	VF_{3-6}
lSc (4)	VF_{4-1}	VF_{4-2}	VF_{4-3}	0	VF_{4-5}	VF_{4-6}
arc (5)	VF_{5-1}	VF_{5-2}	VF_{5-3}	VF_{5-4}	0	VF_{5-6}
electrode (6)	VF_{6-1}	VF_{6-2}	VF_{6-3}	VF_{6-4}	VF_{6-5}	0

View factor matrix.

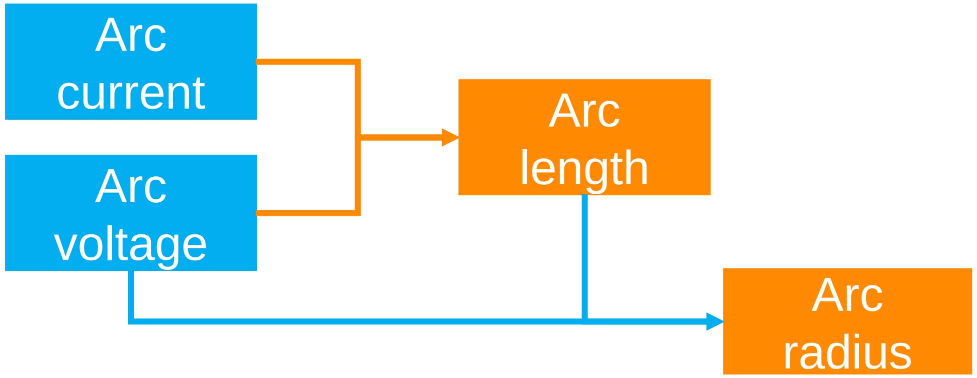
A. Ringel, Master's thesis, RWTH Aachen University, 2020.

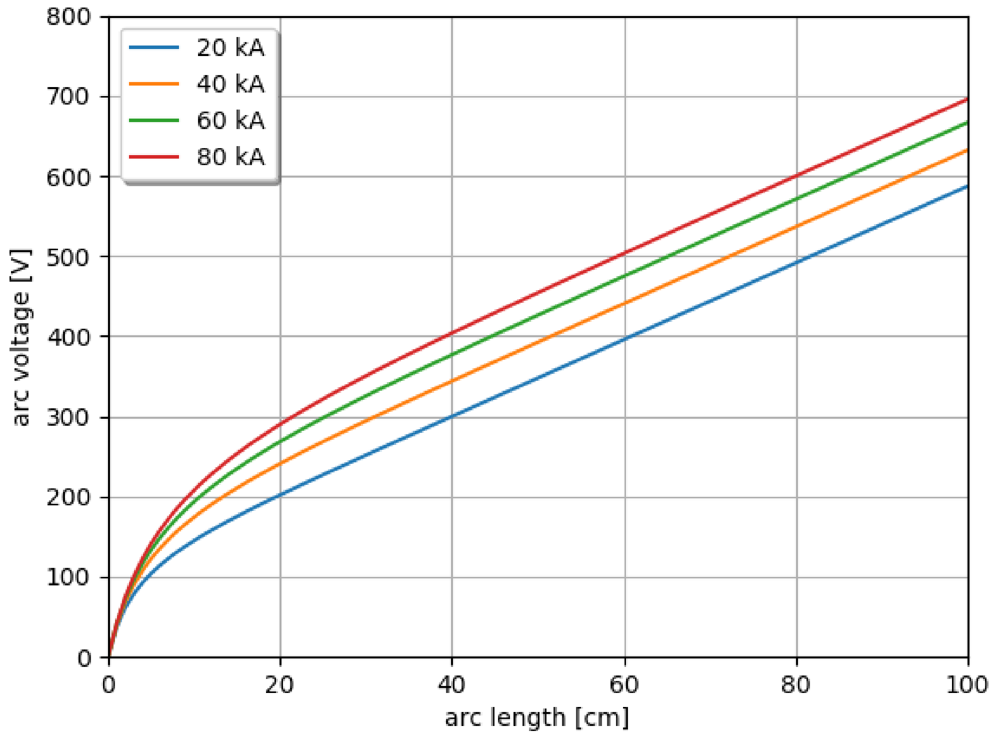
Structure of the model

Scrap melting module

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].





Arc voltage as a function of arc length.
A. Ringel, Master's thesis, RWTH Aachen University, 2020.

References
[1] B. Bowman, "Properties of Arcs in DC Furnaces", 1994.
[2] R. T. Jones et al., Miner. Eng., 15(11): 985–991, 2002.

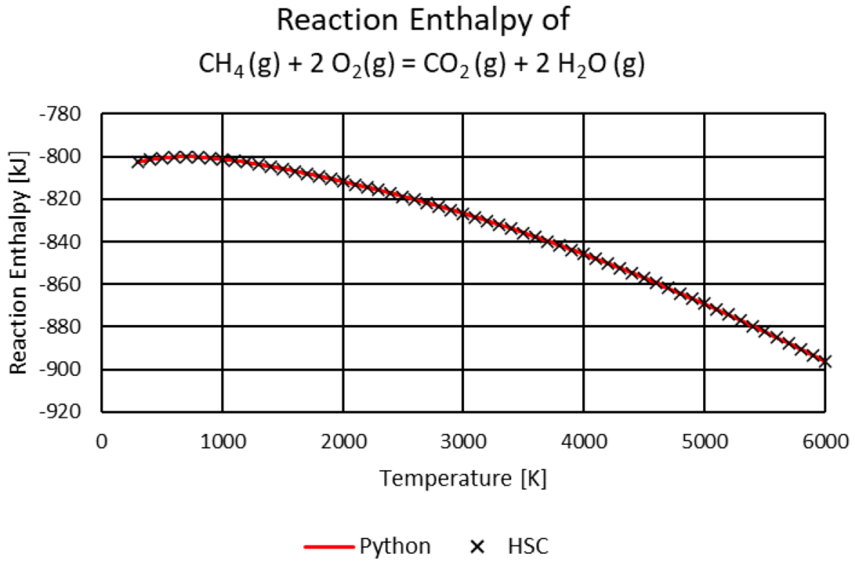
Structure of the model

Scrap melting module

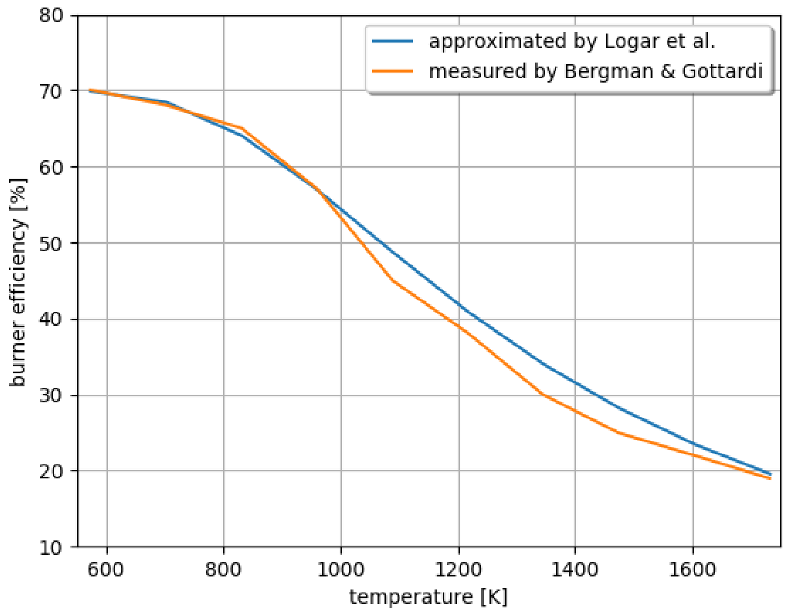
Burners

- The natural gas injected is assumed to be pure methane (CH_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
A. Ringel, Master's thesis, RWTH Aachen University, 2020.



Burner efficiency as a function of temperature.
A. Ringel, Master's thesis, RWTH Aachen University, 2020.



References
[1] K. Bergman & R. Gottardi, Ironmak. Steelmak., 17(4): 282–287, 1990.
[2] Y. N. Toulouevski et al., "Innovation in Electric Arc Furnaces", 2010.
[3] V. Logar et al., ISIJ Int., 52(3): 402–412, 2012.

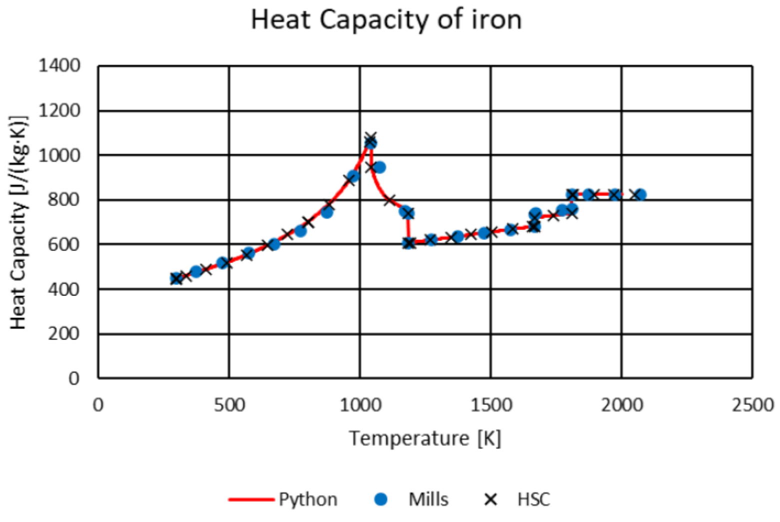
Structure of the model

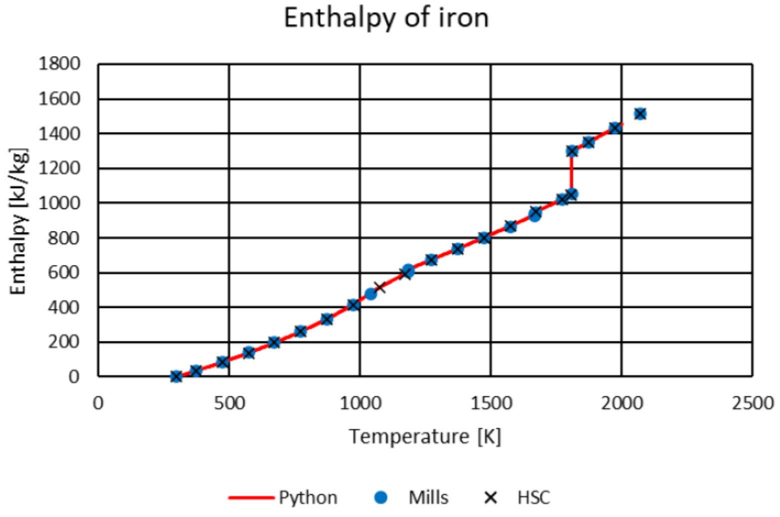
Scrap melting module

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:

Metal	Slag	Gas
Fe, C, Si, Cr, Mn, P	FeO, SiO_2, Cr_2O_3, MnO, P_2O_5, CaO, MgO, Al_2O_3	N_2, O_2, CO, CO_2, CH_4





Specific heat capacity and enthalpy of iron.
A. Ringel, Master's thesis, RWTH Aachen University, 2020.

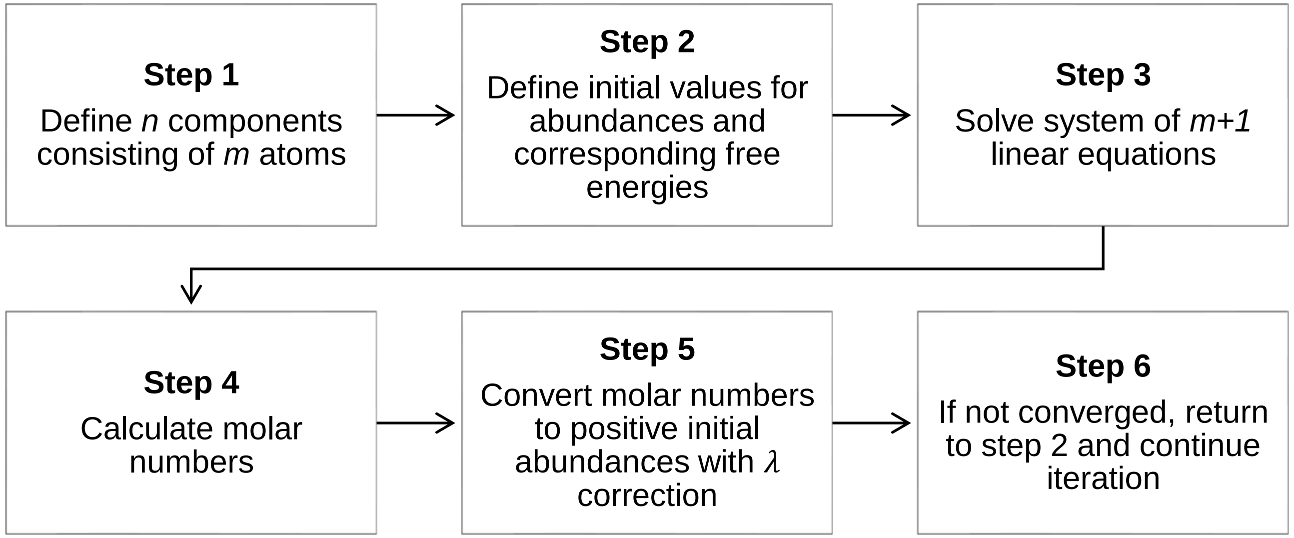
Reference
[1] V.-V. Visuri et al., Proc. ESTAD 2019, 2019.

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.



Execution of the steepest descent method.
Modified from R. Jussila, Master´s thesis, University of Oulu, forthcoming.

References
[1] R. Jussila, Master´s thesis, University of Oulu, forthcoming.
[2] W. B. White, J. Chem Phys. 28(5), 751-755, 1958.
[3] J. Blecic et al., Astrophys. J., Suppl. Ser. 225(1), 2016

Structure of the model

Metal–slag reaction module

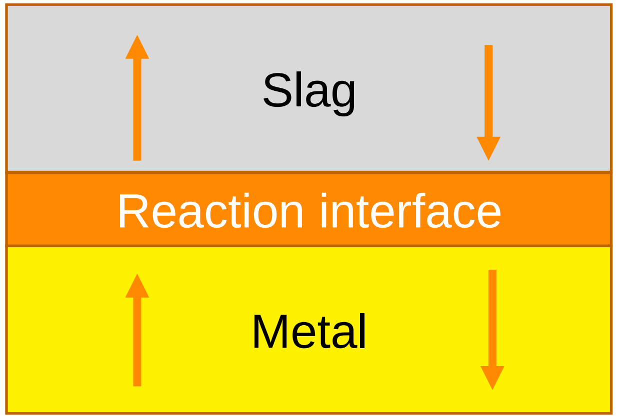
Working principle

- 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

$$J_M = \frac{\beta_{\mathrm{L}}\rho_{\mathrm{L}}}{100M_M}\left([\%M]-[\%M]^*\right) \qquad \text{(in metal)}$$

$$= \frac{\beta_{\mathrm{S}}\rho_{\mathrm{S}}}{100M_{MO_x}}\left((\%MO_x)^*-(\%MO_x)\right) \qquad \text{(in slag)}$$



Electronegativity equation at the interface

$$\sum_{M=1}^{n} J_M \nu_{M,\mathrm{O}} = 0$$

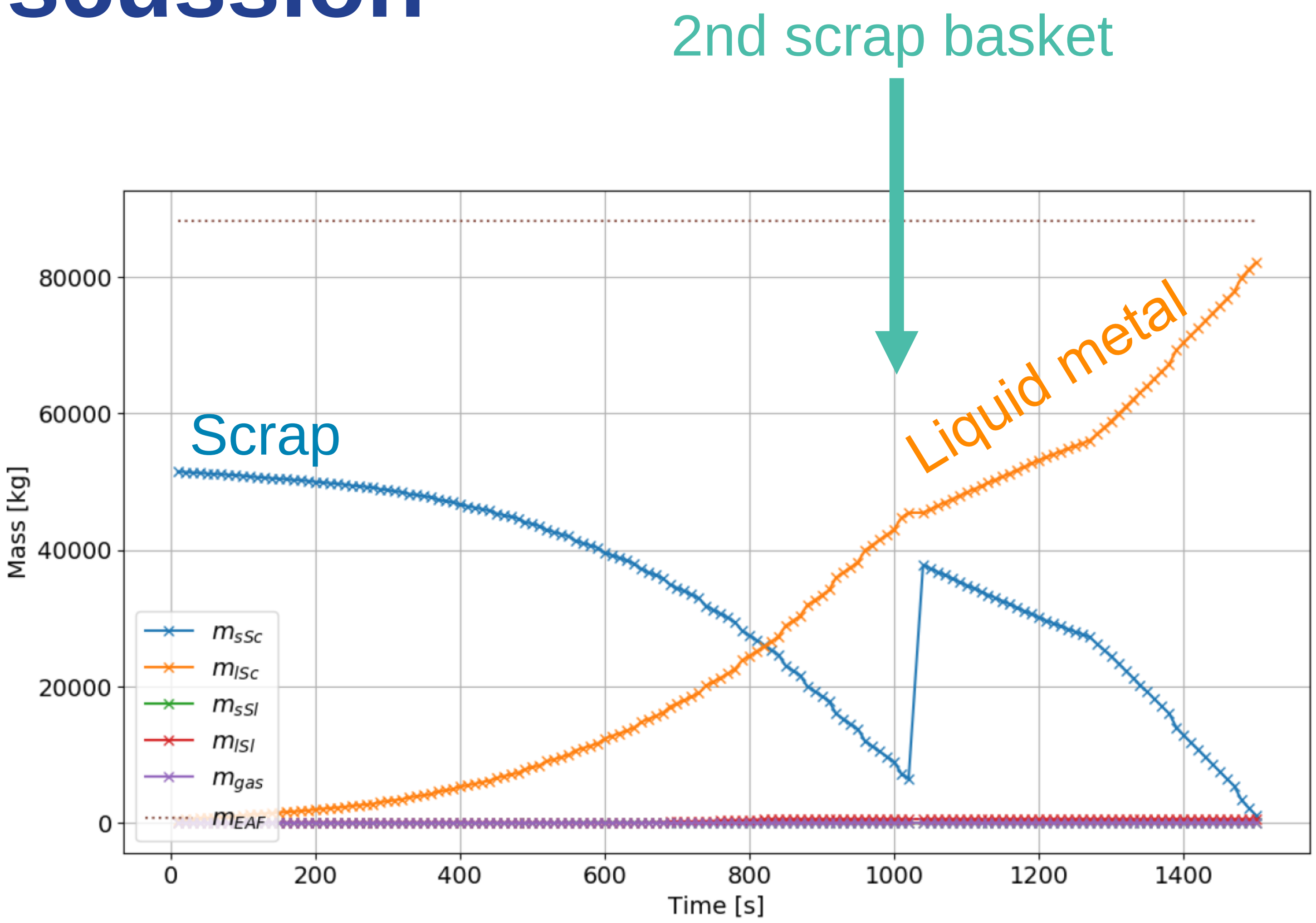
References
[1] L. Hekkala, Master´s thesis, University of Oulu, forthcoming.
[2] D. Robertson et al., Ironmaking Steelmaking, 11(1): 41–55, 1984.
[3] A. D. Pelton and C. W. Bale, Metall. Trans. A, 17(7): 1211-1215, 1986.
[4] S. Ban-Ya, ISIJ Int., 33(1): 2–11, 1993.

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.
A. Ringel, Master's thesis, RWTH Aachen University, 2020.

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.

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

	Study			Error in abundance vs Jussila [1]	
Species	Jussila [1]	White et al. [2]	Blecic et al. [3]	White et al. [2]	Blecic et al. [3]
H	0.040655	0.040668	0.040655	-0.000013	0
H_2	0.147710	0.147730	0.147710	-0.000020	0
H_2O	0.783187	0.783153	0.783187	0.000034	0
N	0.001414	0.001414	0.001414	0	0
N_2	0.485248	0.485247	0.485248	0.000001	0
NH	0.000693	0.000693	0.000693	0	0
NO	0.027397	0.027399	0.027397	-0.000002	0
O	0.017941	0.017947	0.017941	-0.000006	0
O_2	0.037309	0.037314	0.037309	-0.000005	0
OH	0.096857	0.096872	0.096857	-0.000015	0

Virtually no error

References
[1] R. Jussila, Master´s thesis, University of Oulu, forthcoming.
[2] W. B. White, J. Chem Phys. 28(5), 751-755, 1958.
[3] J. Blecic et al., Astrophys. J., Suppl. Ser. 225(1), 2016

Results and discussion

Further work

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?

Collaborators	Topics
Luxmet Oy	Control systems for EAF OES measurements
RWTH Aachen University	Modelling methodology Heat transfer Laboratory experiments
Ovako Imatra Oy	Scrap-based carbon steelmaking
Outokumpu Stainless Oy	Scrap-based stainless steelmaking Alternative EAF technologies

Reference
[1] S. Ohguchi et al., Ironmaking Steelmaking, 11(4): 202-213, 1984.

Results and discussion

Further work

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.

Acknowledgements

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Thank you for your attention!

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