

Coupled dynamic modeling of scrap melting and gas phase reactions in the electric arc furnace process

I Mäkelä¹, V-V Visuri¹, M Aula² and T Echterhof³

¹ Process Metallurgy Research Unit, University of Oulu, PO Box 4300, 90014 University of Oulu, Finland

² Outokumpu Stainless Oy, Terästie, 95400 Tornio, Finland

³ Department for Industrial Furnaces and Heat Engineering, RWTH Aachen University, 52074 Aachen, Germany

ilpo.makela@oulu.fi

Abstract. Gas phase reactions have a significant effect on the composition and heat content of the off-gas in the electric arc furnace (EAF) process. In this work, a previously developed dynamic scrap melting and heat transfer model was coupled with a gas phase reaction module based on Gibbs energy minimization. The gas phase reaction module retrieves the necessary thermodynamic data from a previously developed thermochemistry module. The gas phase reaction module has been used to improve the description of the gas burners and the freeboard of the EAF. The implementation of the gas phase reaction module has been found to be in good agreement with commercially available software (HSC Sim) for calculations assuming a gas phase equilibrium.

1. Introduction

The state of the gas phase within the electric arc furnace (EAF) is an important factor when calculating the energy balance and efficiency of the process. Oxygen in the leakage air or lancing can react with unburnt components of the gas phase, but this leakage air can also cause significant cooling and heat loss in the process. Additionally, the outflow of gases, whether through the hood or gaps in the furnace, can remove significant amounts of unreacted components that could otherwise have contributed to heating the process. Monitoring the gas phase can also provide valuable insight into the progress of the melting and refining processes. Due to these factors, including the gas phase in EAF process modeling is an important issue to consider.

Hay et al. [1] have done an extensive review of fast and comprehensive EAF process models. In their review, it is found that most of the models developed in the last 10 years are based on the works of Logar et al. [2–7], or developed in cooperation with them. The description of the gas phase equilibria in these models mainly considers the combustion of CH₄ and CO, the water-gas shift reaction, the Boudouard reaction and the reaction of C₉H₂₀ with C. These reactions are mainly modeled with the equilibrium constant method.

MacRosty and Swartz [8] modeled the gas phase as a zone where all the components are assumed to exist in a state of chemical equilibrium, which is calculated using the Gibbs free energy minimization



method. The limiting factor of reactions is the mass transfer between the different zones, with the mass transfer coefficient being an adjustable parameter, which can be estimated from industrial data. Mass transfer in the gas phase considers the burners, leakage air, off-gas, electrode cooling with water and transfer occurring between the slag-metal interaction zone. The direction of the leakage air is related to the furnace pressure, but some amount of off-gas seems to always be removed.

The model developed by Meier et al. [9] is based on the model developed by Logar et al. [4,5], with an enhanced description of the off-gas. Meier pointed out that significant amounts of H₂O, H₂ and even CH₄ are measured in the off-gas, and therefore these were included in their model. In Logar's model these components were not included in the gas phase, and complete combustion of CH₄ was assumed. Meier uses equilibrium constants to calculate some of the reaction rates. These equilibrium constants were assumed to only be temperature dependent and were pre-calculated for a range of temperatures for each of the equilibrium reactions to improve model performance. Leak air calculation was done using relative furnace pressure and a constant relating the pressure to the mass flow rate.

The model developed by Hay et al. [10] is based on the model developed by Meier. In their work, Hay pointed out that their pressure calculation within the furnace is unstable, and can start to oscillate, which in turn can slow down or even crash the simulation. This oscillation is caused by a feedback loop from the coupling of the leak air ingress with the pressure and temperature calculations. To counteract this, Hay used empirically derived equations that allowed the model to detect steep changes in the leak airflow and adjust the time step to avoid oscillations.

Our aim is to improve the description of the gas phase. By applying the Gibbs energy minimization method to the description of the gas phase reactions, we could improve the overall accuracy and ease of implementation of even complex gas mixtures. The method does not require the user to define the occurring reactions and their stoichiometries, so implementing new burner gases and accounting for side reactions is quite simple. Additionally, the method inherently considers the interactions between the reactions, while the equilibrium constant method minimizes the Gibbs energy only for individual reactions. In the present paper, we describe the coupling of the previously developed gas phase reaction module [11] and dynamic EAF scrap melting and heat transfer module [12]. The long-term goal is to also consider and implement kinetics into the gas phase modeling for more accurate results.

2. Materials and methods

The scrap melting and heat transfer module originally developed by Ringel [12] is based on previous EAF model work by Logar et al. [3–5], Meier [13] and Fathi [14], and focuses on describing the scrap melting and heat transfer processes. The model uses the explicit Runge-Kutta-Fehlberg method to find the solution using adaptive time-steps. The model reads process data to determine the electrical energy and burner energy inputs, which are then distributed according to a calculated heat transfer matrix. This energy distribution is then used to calculate the change of temperature in different zones as well as the change in mass of solid scrap, melt, slag, etc. In the original implementation, the conversion of the gas burner was assumed to be 100%, and the use of the gas burner did not change the composition of the gas phase, which was simplified to be at the composition of normal atmospheric air. The heat from the burner is transferred to the solid and liquid scrap and the gas phase according to a hyperbolic-tangent approximation also used by Logar et al. [4]:

$$Q_{\text{CH}_4\text{-sSc}} = Q_{\text{r-CH}_4} K_{\text{burn}} \left[0.35 + 0.65 \tanh \left(\frac{1300^\circ\text{C}}{T_{\text{sSc}} - 273.15\text{K}} - 1 \right) \right] \quad (1)$$

$$Q_{\text{CH}_4\text{-gas}} = Q_{\text{r-CH}_4} \left\{ 1 - K_{\text{burn}} \left[0.35 + 0.65 \tanh \left(\frac{1300^\circ\text{C}}{T_{\text{sSc}} - 273.15\text{K}} - 1 \right) \right] \right\} \quad (2)$$

where $Q_{\text{CH4-sSc}}$ is the heat transfer to the scrap [W], $Q_{\text{CH4-gas}}$ is the heat transferred to the gas phase [W], $Q_{\text{r-CH4}}$ is the heat released in the burning [W], K_{burn} is burner efficiency, which is approximated to be 0.7 based on Ref. [15], and T_{sSc} is the temperature of the solid scrap [K].

The gas phase reaction module developed by Jussila [11] uses the minimization of Gibbs energy method, described by White et al. [16] The minimization method retrieves the Gibbs energy data for the species involved from our thermochemistry module. In addition to participating gas species, initial amounts, temperature, and pressure, the equilibrium module can be given a parameter to limit the portion of the input gases, that partake in the equilibrium calculation. By adjusting this parameter, we can force the model to decrease the maximum conversion achieved. In practice this is done by multiplying the molar input values by the limit parameter, which ranges between 0 to 1 for each molecule, and this portion is then fed to the equilibrium calculation routine. The leftover moles of the previous multiplication pass the equilibrium calculation, effectively making them passive from the reactions' standpoint. The leftover moles are then summed with the equilibrated moles to get the final molar amounts.

The thermochemistry module developed originally in C++ in Ref. [17] was converted to Python in Ref. [12] to provide thermochemical properties of different species and their mixtures, as well as reactions at a range of temperatures. The module retrieves tabulated data such as the Shomate coefficients, standard enthalpy and standard entropy from a csv file, and processes this into a Python dictionary, from which the equations (functions) can then retrieve the needed data with species name, temperature, and property index as parameters. If thermochemical data is not available for a given temperature, the model extrapolates using the last available values, though for the present work, we have enough data to cover the operating temperatures of the EAF. For calculating the Gibbs energies, the thermochemistry module uses the following equations:

$$C_p = A + B \cdot T \cdot 10^{-3} + C \cdot T^2 \cdot 10^5 + D \cdot T^2 \cdot 10^{-6} + E \cdot T^{-3} \cdot 10^8 + F \cdot T^3 \cdot 10^{-9} \quad (3)$$

$$\Delta H = H_{298.15}^{\circ} + \int_{298.15}^T C_p dT + \sum H_{\text{tr}} \quad (4)$$

$$\Delta S = S_{298.15}^{\circ} + \int_{298.15}^T \frac{C_p}{T} dT + \sum S_{\text{tr}} \quad (5)$$

$$\Delta G = \Delta H - T\Delta S \quad (6)$$

where C_p is the molar heat capacity [$\text{J K}^{-1} \text{mol}^{-1}$], A through F are coefficients for the Shomate equation, ΔH is the molar enthalpy at temperature T [J mol^{-1}], $H_{298.15}^{\circ}$ is the standard enthalpy [J mol^{-1}], $\sum H_{\text{tr}}$ is the enthalpy associated with phase transformations occurring between temperatures 298.15 K and T [J mol^{-1}], ΔS is the molar entropy at temperature T [$\text{J K}^{-1} \text{mol}^{-1}$], $S_{298.15}^{\circ}$ is the standard entropy [$\text{J K}^{-1} \text{mol}^{-1}$], $\sum S_{\text{tr}}$ is the entropy associated with phase transformations occurring between temperatures 298.15 K and T [$\text{J K}^{-1} \text{mol}^{-1}$] and ΔG is Gibbs energy at temperature T [J mol^{-1}].

The implementation of the gas burner from Logar et al. [4,5] was modified by using the gas phase equilibrium module to calculate the equilibrium composition of the gas leaving the burner, and the energy released in the reactions. This allows us to model the conversion of the burner and possible side reactions with a relatively simple implementation. The calculation routine takes the possible gas species present in the burner region, the fuel gas feed rate, and gas phase temperature as inputs. It then calculates the stoichiometric amount of oxygen needed for complete burning of the fuel gas and adds it to the reaction. The module then calculates the equilibrium at the given gas phase temperature, and the change in enthalpy to find the energy released, which is then divided between the scrap and the gas phase according to equations (1) and (2). The calculation also gives the feed rate for output gases, which are added to the gas phase according to the taken time step size in the solver. The implementation allows

for a quick and easy way to change the used fuel and lambda (supplied amount of oxygen compared to the stoichiometric amount of oxygen) in the simulation.

The equilibrium module was also implemented to consider the whole freeboard gas phase of the EAF. In its current implementation, the gas phase is treated as an adiabatic equilibrium reactor. The model uses the secant method to find a temperature and composition where the error between the initial and final enthalpy is below the set tolerance. The leakage air is adjusted by calculating the maximum amount of gas that can be present in the freeboard, using the ideal gas law, and comparing this with the current amount of gas in the calculation. If there is more gas than the freeboard can contain in its current conditions, the excess leaks out, but if there is less gas, air leaks in diluting the composition and lowering its temperature, further increasing the amount of gas leaking in. The balance between the new temperature and air intake is solved using the secant method. The calculation routine is illustrated in figure 1. The present implementation enables initial testing on the gas phase module. In further work, it would be relevant to modify the model to account for a pressure-driven gas flow to obtain more realistic results.

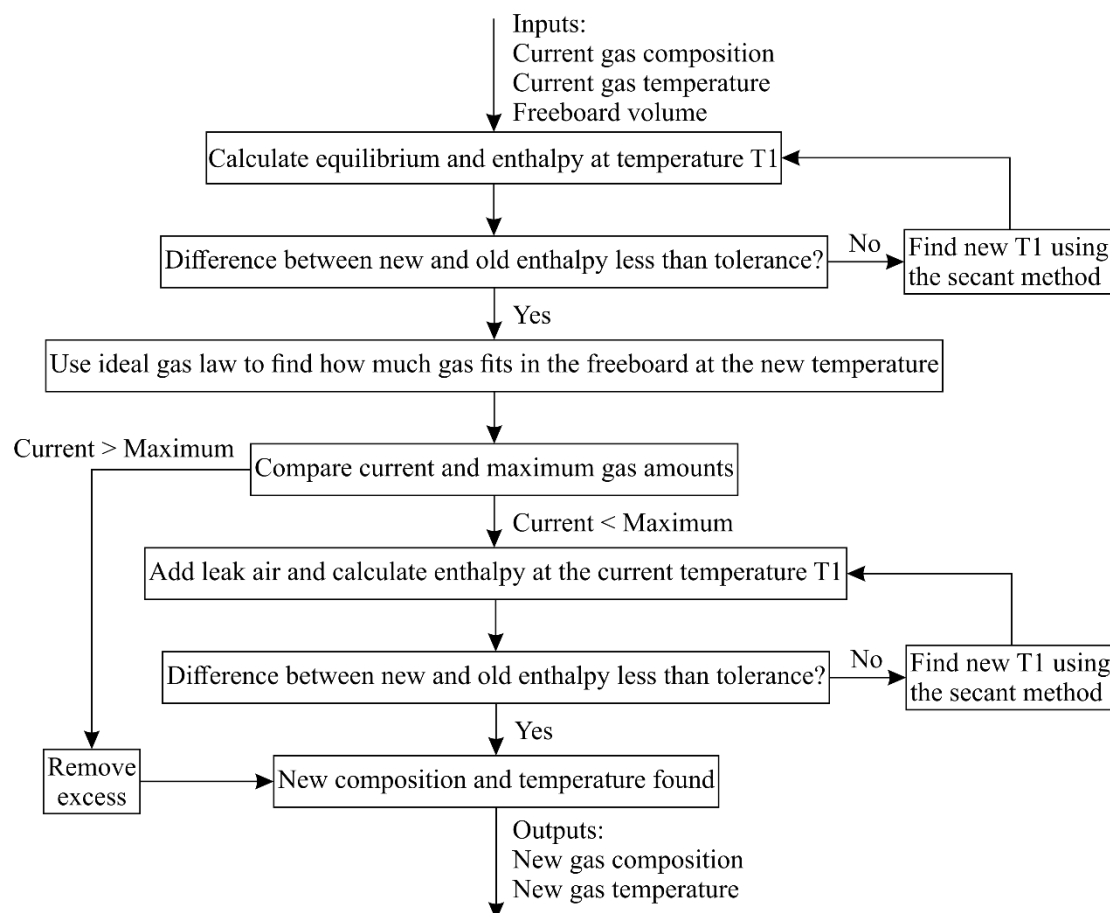


Figure 1. Gas phase calculation routine.

3. Results

Our implementation of the gas phase equilibrium calculation was compared with the HSC Chemistry 10 (version 10.0.7.13) Sim module equilibrium calculation, through the burning of methane. If the amount of some gas specie(s) reaches zero in the simulation, it can lead to the model trying to calculate the natural logarithm of zero at these points. To counteract this, the model checks for these zero values, and replaces them with a very small value of 10^{-10} moles. All the following simulations were performed on

an laptop with 11th Gen Intel(R) Core(TM) i5-1135G7 @ 2.40GHz processor and Windows 10 64-bit operating system.

The simulated burner was fed with 10 moles of CH₄ and 500 moles of air (79 mol-% N₂, 21 mol-% O₂) at 1500 °C (1773.15 K). The output species specified for the system were N₂, O₂, CH₄, CO, CO₂, H₂O_(g) and H₂, while the temperature of the output was controlled so that an energy balance was achieved between the inputs and outputs. The results of the simulations are presented in table 1. The results of the simulations using the HSC Sim and Python models are in nearly perfect agreement. The gas phase compositions are almost identical, and the temperature difference is only 0.40 °C, while the increase in temperature was around 422 °C.

For the studied system, the calculation time to find the equilibrium composition and temperature was approximately 0.8 s using an error tolerance of 10⁻⁵ J. The input and output states are far apart, meaning longer calculation times to find the equilibrium. When the input and output states are close together, for example in a simulation where the modeled gas phase changes little between taken time steps, the calculation times can be assumed to be much faster. HSC is generally able to find the equilibriums much faster than our Python model, however, HSC cannot be coupled with the Python model or used in online process modeling.

Table 1. Equilibrium calculation for HSC sim model and Python model.

Property	Unit	Input	Output	
			HSC sim model	Python model
CH ₄	mol	10	0	6.70·10 ⁻²⁰
N ₂	mol	395	395.00	395.00
O ₂	mol	105	85.11	85.10
CO	mol	0	0.14	0.14
CO ₂	mol	0	9.86	9.86
H ₂ O _(g)	mol	0	19.94	19.95
H ₂	mol	0	0.054	0.054
Temperature	°C	1 500	1922.60	1922.20

Additionally, the sensitivity of the EAF model coupled with the equilibrium module was inspected by adjusting model parameters such as maximum time step size (Δt), and relative and absolute tolerances of the solver. It should be noted that as the model uses adaptive Δt , the modeled points in time are rarely exactly the same, and the compared points need to be chosen so that they are close to each other. Inspecting the table 2, containing the results from adjusting the maximum Δt , decreasing the Δt value below 1 s, seems to change the results very little. Increasing the Δt to 2s changes the temperature by 7.05 K and 8.16 K compared to 1 s Δt , at simulation points 920 s and 2 000 s respectively. In tables 3 and 4, we have compiled the results from adjusting the relative and absolute tolerances of the solver. Decreasing the tolerance values below 1 changes the results of the model very little. It was chosen that 1 s Δt , and tolerance values of 1 are adequate for the use of the model.

Table 2. Model gas phase sensitivity to the Δt size, with tolerance values set to 1.

max Δt	Model time (s)	Gas temperature (K)	Mass of gas (kg)	CO ₂ amount (mol)
2.0 s	920.67	1 378.06	12.89	161.06
1.0 s	919.99	1 385.11	12.82	159.47
0.5 s	920.01	1 384.47	12.84	159.69
0.2 s	920.09	1 384.24	12.84	159.76
2.0 s	2 000.71	1 475.78	10.91	136.20
1.0 s	2 000.14	1 483.94	10.86	135.19
0.5 s	2 000.24	1 480.37	10.88	135.75
0.2 s	2 000.16	1 480.75	10.88	135.66

Table 3. Model gas phase sensitivity to the relative tolerance of the solver, with $\Delta t = 1$ s and absolute tolerance set to 1.

Relative tolerance	Model time (s)	Gas temperature (K)	Mass of gas (kg)	CO ₂ amount (mol)
1.0	919.99	1 385.11	12.82	159.47
0.5	919.99	1 385.17	12.82	159.47
0.2	920.10	1 383.79	12.84	159.70
1.0	2 000.14	1 483.94	10.86	135.19
0.5	2 000.17	1 483.74	10.86	135.13
0.2	2 000.15	1 483.56	10.85	135.09

Table 4. Model gas phase sensitivity to the absolute tolerance of the solver, with $\Delta t = 1$ s and relative tolerance set to 1.

Absolute tolerance	Model time (s)	Gas temperature (K)	Mass of gas (kg)	CO ₂ amount (mol)
1.0	919.99	1 385.11	12.82	159.47
0.5	919.79	1 385.05	12.82	159.69
0.2	919.97	1 385.13	12.82	159.47
1.0	2 000.14	1 483.94	10.86	135.19
0.5	2 000.18	1 483.81	10.86	135.13
0.2	1 999.90	1 482.04	10.87	135.58

Additionally, the effect of adjusting the conversion of the burner was studied. This was conducted by decreasing the amount of oxygen supplied with the fuel gas, and by adjusting the limiter parameter. In the first case, the amount of oxygen supplied was reduced to 90% of the amount required for the complete burning of the methane gas. The results are shown in figure 2. The supplied methane first exhausts the oxygen in the gas phase, after which CO and H₂ start to form due to the lack of O₂. The lack of oxygen leads to incomplete combustion of CH₄ according to equation (7):



In this case, however, we would be seeing H₂ to CO rates of 2:1, which is not the case in our simulation. At the beginning, we observe higher than expected amounts of H₂, and at a later stage we observe higher than expected amounts of CO. This can be explained by the water-gas shift reaction shown in equation (8):



It is likely that at the beginning the thermodynamic conditions favor the formation of reaction products (CO_2 and H_2), but as the gas phase temperature rises, the reaction equilibrium shifts to favor the formation of reactants (CO and H_2O). However, we need to state that we don't know the exact reactions occurring in our system, as defining them is not needed for calculating the equilibrium compositions using the Gibbs energy minimization method.

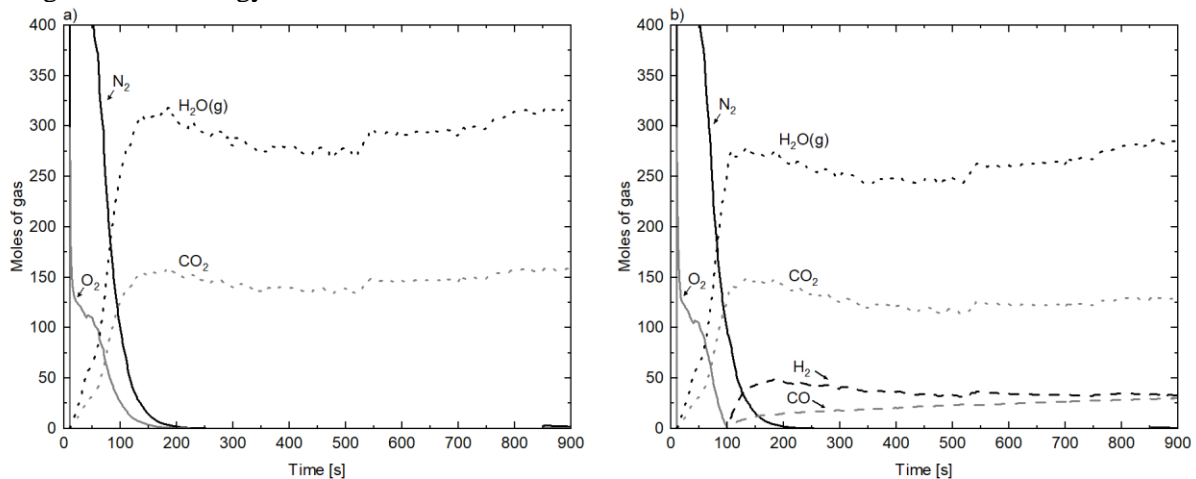


Figure 2. Composition of the gas phase when the burner is supplied with a) stoichiometric amount of oxygen, b) 90% of the stoichiometric amount of oxygen.

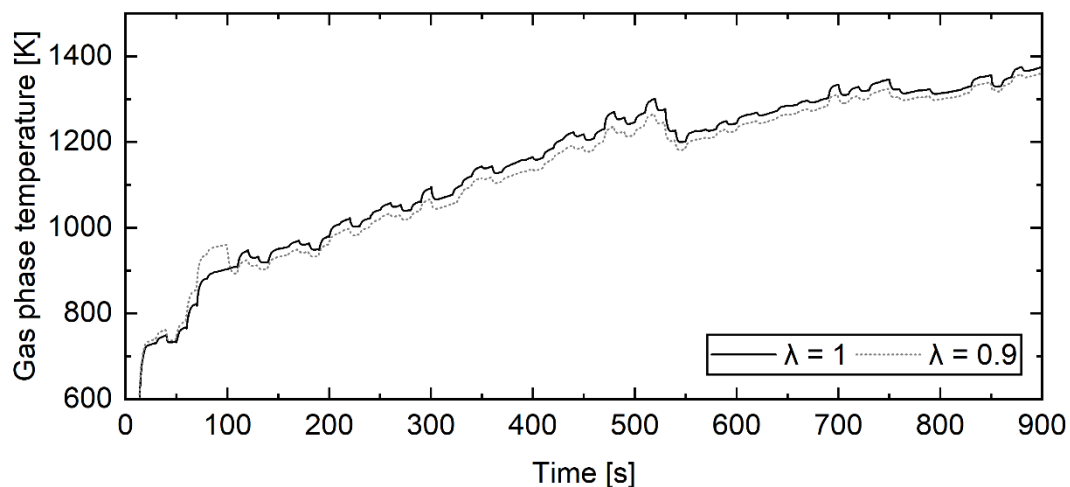


Figure 3. Gas phase temperature when the burner is supplied with stoichiometric amount of oxygen ($\lambda = 1$) and 90% of the stoichiometric amount of oxygen ($\lambda = 0.9$)

Also, the temperature of the gas phase was on average 16 K hotter in the case with stoichiometric amount of oxygen, as shown in figure 3. In the figure we can also see that at the beginning the gas phase is significantly hotter in the case with limited oxygen supply. This is caused by the way that heat is distributed in the burner calculation and will be expanded upon in the following paragraph.

When the burner was supplied with a stoichiometric amount of oxygen, but the reaction was limited to 75% conversion, the gas phase was found to be generally hotter than in the case with 100% burner conversion (see figure 4). This can be attributed to the way that the energy from the burning is divided. When the methane is burned in the burner, the energy is divided between the gas phase and the metal. However, when the combustion is not complete, but we supply the furnace with the required oxygen, the methane reacts in the freeboard gas phase equilibrium calculation, where the energy is not divided,

instead staying in the gas phase and then transferred to the other parts of the furnace according to the heat transfer matrix. This is also what happens at the beginning of our previous example ($\lambda = 0.9$ in figure 3), where some of the burner gases react with the oxygen in the freeboard.

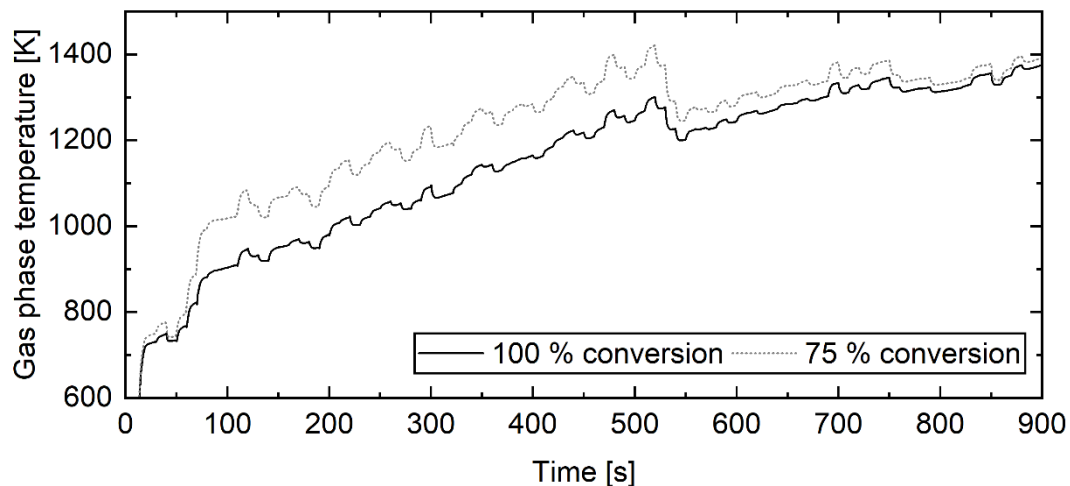


Figure 4. Gas phase temperature comparison

4. Discussion

The implementation of the gas phase reaction module has allowed the previously developed scrap melting and heat transfer module to also consider the composition and reactions of the gas phase, with a relatively simple implementation. The implementation however requires further improvements for more realistic modeling results, especially for the description of the leakage air. Currently, the leakage air is modeled in a way, that rarely allows air to leak in, hindering some reactions and the heat losses caused by this leakage air. The implementation also neglects to consider the kinetics of gas phase reactions, instead assuming the gas phase to always be in a state of equilibrium.

Using the gas phase reaction module at each taken time-step also increases the computation time to a degree where the model is not usable in online process modeling applications. To improve the computation times, either the gas phase reaction module needs to be optimized to find the equilibrium faster, or its use frequency needs to be lowered. The implementation could be further improved by having the gas phase reaction module find the equilibrium after pre-determined time steps or changes in the system and have reaction kinetics then drive the composition towards the found equilibrium.

5. Conclusions

The present paper describes the first implementation of coupling previously developed models for scrap melting and gas phase reactions. The implementation allows a more detailed description of the gas phase composition and the reactions occurring in it. The results obtained using the gas phase reaction module were found to be in excellent agreement with commercially available software. Sensitivity analysis indicates that the coupled model is sufficiently robust for process modeling. As for further work, the recommended improvements include the implementation of reaction kinetics, improvements to the implementation of the leakage air, and optimization of the equilibrium calculation and its implementation.

6. Acknowledgements

This work was conducted within the framework of the Towards Fossil-Free Steel (FFS) project funded by Business Finland and the Towards CO₂-lean electric arc furnace steelmaking through fundamental and data-driven mathematical modeling (LEAF) project funded by the Research Council of Finland

(project no. 356439). Furthermore, Technology Industries of Finland Centennial Foundation Steel and Metal Producers' Fund is gratefully acknowledged for the financial support of Ilpo Mäkelä.

References

- [1] Hay T, Visuri V-V, Aula M and Echterhof T 2021 A Review of Mathematical Process Models for the Electric Arc Furnace Process *Steel Res Int* **92** 2000395
- [2] Logar V, Fathi A and Škrjanc I 2016 A Computational Model for Heat Transfer Coefficient Estimation in Electric Arc Furnace *Steel Res Int* **87** 330–8
- [3] Logar V and Škrjanc I 2012 Modeling and Validation of the Radiative Heat Transfer in an Electric Arc Furnace *ISIJ Int* **52** 1225–32
- [4] Logar V, Dovžan D and Škrjanc I 2012 Modeling and Validation of an Electric Arc Furnace: Part 1, Heat and Mass Transfer *ISIJ Int* **52** 402–12
- [5] Logar V, Dovžan D and Škrjanc I 2012 Modeling and Validation of an Electric Arc Furnace: Part 2, Thermo-chemistry *ISIJ Int* **52** 413–23
- [6] Logar V, Dovžan D and Škrjanc I 2011 Mathematical Modeling and Experimental Validation of an Electric Arc Furnace *ISIJ Int* **51** 382–91
- [7] Logar V and Škrjanc I 2012 Development of an Electric Arc Furnace Simulator Considering Thermal, Chemical and Electrical Aspects *ISIJ Int* **52** 1924–6
- [8] MacRosty R D M and Swartz C L E 2005 Dynamic Modeling of an Industrial Electric Arc Furnace *Ind Eng Chem Res* **44** 8067–83
- [9] Meier T, Gandt K, Echterhof T and Pfeifer H 2017 Modeling and Simulation of the Off-gas in an Electric Arc Furnace *Metall Mater Trans B* **48** 3329–44
- [10] Hay T, Echterhof T and Visuri V-V 2019 Development of an Electric Arc Furnace Simulator Based on a Comprehensive Dynamic Process Model *Processes* **7** 852
- [11] Jussila R *Modelling of gas-phase reactions in the freeboard of the EAF* Unpublished master's thesis (Oulu: University of Oulu)
- [12] Ringel A 2020 *Online modelling of an electric arc furnace* Master's thesis (Aachen: RWTH Aachen university)
- [13] Meier T 2016 *Modellierung und Simulation des Elektrolichtbogenofens* PhD Thesis (Aachen: RWTH Aachen university)
- [14] Fathi A, Saboohi Y, Škrjanc I and Logar V 2017 Comprehensive Electric Arc Furnace Model for Simulation Purposes and Model-Based Control *Steel Res Int* **88** 1600083
- [15] Toulouevski Y N and Zinurov I Y 2013 *Innovation in Electric Arc Furnaces* (Springer)
- [16] White W B, Johnson S M and Dantzig G B 1958 Chemical Equilibrium in Complex Mixtures *J Chem Phys* **28** 751–5
- [17] Visuri V-V, Sulasalmi P, Vuolio T, Paananen T, Haas T, Pfeifer H and Fabritius T 2019 Mathematical Modelling of the Effect of Reagent Particle Size Distribution on the Efficiency of Hot Metal Desulphurisation *Proceedings of the 4th European Steel Technology and Application Days* (Düsseldorf, Germany)