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authored by T. Meier, K. Gandt, T. Echterhof, H. Pfeifer

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Department for Industrial Furnaces and Heat Engineering
RWTH Aachen UniversityWebsite: www.iob.rwth-aachen.de/en/
E-mail: contact@iob.rwth-aachen.deKopernikusstr. 10Phone: +49 241 80 2593652074 Aachen, GermanyFax: +49 241 80 22289

1	Modeling and Simulation of the Off-Gas in an Electric Arc Furnace
2	
3	Thomas Meier, Karima Gandt, Thomas Echterhof, Herbert Pfeifer
4	Corresponding author: Thomas Echterhof, email: echterhof@iob.rwth-aachen.de
5	
6	RWTH Aachen University
7	Department for Industrial Furnaces and Heat Engineering
8	Kopernikusstrasse 10
9	52074 Aachen
10	Germany
11	

12 Keywords:

13 EAF; off-gas modeling; chemical reaction modeling

14 Abstract:

15 The following paper describes an approach to process modeling and simulation of the gas phase in an electric arc furnace (EAF). The work presented represents the continuation of research by 16 17 Logar, Dovžan and Škrjanc on modeling the heat and mass transfer and the thermochemistry in 18 an EAF. Due to the lack of off-gas measurements, Logar et al. modeled a simplified gas phase 19 under consideration of five gas components and simplified chemical reactions. The off-gas is 20 one of the main continuously measurable EAF process values and the off-gas flow represents a 21 heat loss up to 30% of the entire EAF energy input. Therefore, gas phase modeling offers further 22 development opportunities for future EAF optimization. This paper presents the enhancement 23 of the previous EAF gas phase modeling by the consideration of additional gas components and 24 a more detailed heat and mass transfer modeling. In order to avoid the increase of simulation 25 time due to more complex modeling, the EAF model has been newly implemented to use an 26 efficient numerical solver for ordinary differential equations (ODE). Compared to the original 27 model, the chemical components H₂, H₂O and CH₄ are included in the gas phase and equilibrium reactions are implemented. The results show high levels of similarity between the 28 29 measured operational data from an industrial scale EAF and the theoretical data from the 30 simulation within a reasonable simulation time. In the future, the dynamic EAF model will be 31 applicable for on- and offline optimizations, e.g. to analyze alternative input materials and mode 32 of operations.

33

34 **1. Introduction**

35 Electric steelmaking in an electric arc furnace (EAF) is the main process route for steel scrap recycling and the second most important steel production route in the world. As an energy-36 37 intensive process, the EAF is responsible for approximately 3% of the total industrial electricity consumption and a significant lever for energy efficiency optimization [1]. As the off-gas flow 38 39 represents an energy output of 20-30% of the total EAF energy input, the off-gas is in the focus 40 of current developments to increase the energy and resource efficiency of the EAF. As one of 41 the main continuously measurable process values, the off-gas composition can be utilized to improve the process control and allows conclusions to be made concerning the process behavior. 42 43 Here, process models have proven their applicability for process control and their capability to 44 contribute towards a more detailed understanding of heat and mass transfer during the melting 45 process. In times of continuously growing computational capacity, the complexity of the 46 dynamic process simulation models has increased due to the consideration of more and more 47 phenomena. Logar et al. [2-4] presented a comprehensive deterministic EAF model, which is 48 based on fundamental physical and mathematical equations. The model includes all main 49 thermal, chemical and mass transfer phenomena in the EAF. These are implemented via first order ordinary differential equations (ODE). It was further developed and enhanced with a more 50 51 detailed simulation of the arc heat distribution and a modified chemical module [5, 6]. Due to 52 the lack of off-gas data from the validation furnace, the gas phase was simplified. Five chemical 53 components are taken into account and chemical reactions are only considered for post-54 combustion. As one of the best recently published EAF models, it was found to be suitable a 55 starting point for further development of the gas phase modeling, which is described within this 56 paper, which is therefore a continuation of the work done by Logar et al.

A detailed literature review shows that there are other papers addressing the modeling of the gas phase in an EAF, but with different approaches and simplifications. Opitz and Treffinger [7] use the model of Logar et al. to design a dynamic, physics-based model of a complete EAF 60 plant which consists of four sub-systems (vessel, electric system, electrode regulation and off-61 gas system). Matson and Ramirez [8, 9] consider six chemical elements in the off-gas and determine the reaction rates with a chemical equilibrium algorithm by Gibbs free energy 62 63 minimization. The simulation calculation time is not mentioned and is assumed slow compared to other approaches. Furthermore, the results of the gas phase simulation are not compared to 64 65 measured data and the curves show a constant behavior over long periods. MacRosty and 66 Swartz [10] consider all relevant species in the gas zone and assume chemical equilibrium in 67 each zone. The model does not address gas radiation and requires a high computing capacity. Nyssen et al. [11] published another EAF model. The model seems to include all major 68 69 processes, but no details are given in the publication.

The objective of this work was to consider all major measurable gas components in an EAF process model. Therefore, in addition to CO, CO₂, N₂, O₂, and CH₄ the components H₂, H₂O, and CH₄ are also included in the gas phase of this study. The components are considered in chemical reactions for post-combustion, major equilibrium reactions and dissociation. To prevent the increase of simulation time, the EAF model was newly implemented in MATLAB to use the internal ODE-solver instead of the fixed step Euler method, which was chosen by Logar et al.

The further development is based on an industrial scale 140 t EAF. The operational data of the EAF is used for the model parametrization and final validation of the simulation results. The input powers and mass flows of the periphery is used as input data for the simulation. The simulation results are evaluated concerning off-gas composition, temperature and energy.

81 2. Modeling

Within this section, the approach of modeling the off-gas is described as an enhancement to the EAF process model developed by Logar et al. [2, 3]. Therefore, the paper follows the basic assumptions and simplifications as addressed in part 1 [2] and part 2 [3] of the EAF model

- publication from Logar et al., which are also valid for this enhanced model and will not be
 repeated in this paper. The EAF is divided into eight different zones:
- 87 1. Solid scrap (sSc)
- 88 2. Liquid Scrap (ISc)
- 89 3. Solid slag (sSl)
- 90 4. Liquid slag (ISI)
- 91 5. Gas phase (gas)
- 92 6. Walls (wall)
- 93 7. Electrode/s (el)
- 94 8. Electric arc/s (arc).

95 Each zone and chemical component has assigned physical properties, i.e. specific heat capacity

96 C_p , density ρ , molar mass M etc. The values used for the parameters are listed in the Appendix

97 in **Table 5**.

101

98 Within and between the defined phases inside the EAF vessel, thermo-chemical reactions, as

99 well as heat and mass transfer take place. Figure 1 gives a schematic overview of the enhanced

100 model structure and the basic functioning.



- 102 **Fig. 1.** Structure and functioning of the EAF process model.
- 103 2.1. New Model Implementation

104 To overcome the contradiction between simulation accuracy, simulation calculation time and 105 numerical integration time steps, the EAF model has been newly implemented to use efficient 106 ODE-solving methods within the software MATLAB. While Logar et al. [2] used a fixed step 107 Euler method with a chosen time step of 10^{-4} s, numerical integration methods with a variable 108 calculation of the integration time step have proven their efficiency to solve complex ODE-109 systems [12].

The usage of the MATLAB ODE-solving methods required several model modifications. Sudden changes caused by if-else conditions were replaced by continuous algorithms to realize on/off behavior. In detail, the variable that has to be switched is multiplied with a modified hyperbolic tangent function, which results in values of zero and one with a continuous transition. Furthermore, the calculation of the melting geometry is performed by modeling the scrap heap as a body of revolution around the middle axis of the EAF. A variable angle of the borehole in the scrap is used to determine the geometrical data for the view factor calculation [13].

As a consequence of mass transfer between the different phases, mixing temperatures have to be calculated. Because the step size is not directly known during the simulation, the calculation of the mixing temperature is directly integrated into the calculation of the temperature change rates. In a general way, this is determined according to Eq. (1):

$$\frac{\mathrm{d}T_{xx}}{\mathrm{d}t} = \frac{Q_{xx} - (T_{xx} - T_{addition})C_{p,addition}\dot{m}_{addition}}{m_{xx}C_{p,xx}} \tag{1}$$

121 A phase xx (with mass m_{xx} , temperature T_{xx} and heat capacity $C_{P,xx}$) changes its temperature due 122 to adding a mass (with mass flow $\dot{m}_{addition}$, temperature $T_{addition}$ and heat capacity $C_{P,addition}$) by 123 the temperature rate $\frac{dT_{XX}}{dt}$. The resulting net heat flow is \dot{Q}_{xx} , which is positive or negative, 124 depending on the temperature difference ($T_{xx} - T_{addition}$). One example is the temperature change 125 of the liquid steel melt (ISc), which is calculated according to Eq. (2):

$$\frac{\mathrm{d}T_{lSc}}{\mathrm{d}t} = \frac{1}{m_{lSc}C_{p,lSc}} \left[\dot{Q}_{lSc} - \dot{m}_{solidify} \lambda_{sSc} + (T_{lSc} - T_{melt,sSc}) \dot{m}_{sSc} C_{p,lSc} - (T_{lSc} - T_{air}) (\dot{m}_{o2-lance} C_{p,O2} + \dot{m}_{c-inj} C_{p,C}) \right]$$
(2)

126 where \dot{Q}_{lSc} denotes the net heat flow of the liquid melt, $\dot{m}_{solidify}$ represents a negative mass flow 127 to the scrap if solidification occurs and λ_{sSc} is the latent heat of fusion, \dot{m}_{sSc} is the negative mass 128 change rate of scrap, $\dot{m}_{O2-lance}$ and \dot{m}_{C-inj} are the injection of oxygen and carbon into the melt, 129 and T_i are the corresponding temperatures with the ambient temperature T_{air} .

After the re-implementation, it was found that the ODE-system of the model is stiff. As the multi-step BDF/NDF solver ode15s is most suitable for stiff ODE-systems and delivered best results in terms of accuracy and speed, it was chosen for future developments. Further investigation on numerical solution methods for EAF modeling was done by Meier and Logar

134 [12].2.2. Relevant Chemical Off-Gas Elements

The gas phase (gas) in Logar's model consists of the five elements CO, CO₂, N₂, O₂ and CH₄, where total combustion of CH₄ is assumed [2, 3]. Due to the fact that the H₂O and H₂ mass fractions reach significant values during off-gas composition measurements, whereby CH₄ is detected in the off-gas as well, those elements are considered in the gas phase of the new enhanced EAF model using the following modifications. The mass flows of H₂, H₂O and CH₄ into the EAF and their outflow due to the off-gas removal and blow out are described in the following section as well as the chemical reactions and the reaction enthalpies.

142 **2.3. Chemical Reactions**

A considerable amount of energy is required for steel production. This necessary thermal energy is provided by the electric arcs and by the conversion of chemical energy to thermal energy by oxidation reactions [14]. The oxidizing reactants are mainly provided by the charged coal and the burners. However, there are also smaller amounts of reactants, e.g. due to electrode consumption and contaminants adhering to the scrap, such as paint or plastics. They are assumed to be nonane (C_9H_{20}). Logar et al. [3] defined 15 reactions (a) to (p) ((o) is missing)

- which are occurring in the liquid melt, the liquid slag and the gas phase. The reaction equations
 (a) to (m) were adopted unchanged. The reactions concerning methane (n) and nonane (p) were
 slightly adapted and further reactions (from (q) to (u)) were implemented for the gas phase. The
- 152 altered and added reactions are listed in Eq. (3):

$$(n_{1}) CH_{4} + 2O_{2} \rightarrow CO_{2} + 2H_{2}O$$

$$(n_{2}) 2CH_{4} + 3O_{2} \rightarrow 2CO + 4H_{2}O$$

$$(n_{3}) CH_{4} + O_{2} \rightarrow CO_{2} + H_{2}$$

$$(p) C_{9}H_{20} \rightarrow 9C + 10H_{2}$$

$$(q) CO + H_{2}O \leftrightarrow CO_{2} + H_{2}$$

$$(r) C + CO_{2} \leftrightarrow 2CO$$

$$(s) C + H_{2}O \leftrightarrow CO + H_{2}$$

$$(t) H_{2} + \frac{1}{2}O_{2} \leftrightarrow H_{2}O$$

$$(u) C + \frac{1}{2}O_{2} \rightarrow CO$$

$$(s) C + \frac{1}{2}O_{2} \rightarrow CO$$

$$(s) C + \frac{1}{2}O_{2} \rightarrow CO$$

153 These reactions present the enhancement of the current models gas phase. They mainly effect 154 the rates of change of elements and the calculation of reaction enthalpies. This is addressed in 155 the following section.

156 2.3.1 Equilibrium Reactions

157 Due to the typical temperatures in EAFs between 1273 K and 2273 K (1000 °C and 2000 °C), 158 equilibrium reactions as well as dissociation have to be considered in the modeling of the gas 159 phase. While taking into account the elements of the gas phase and the presence of C in the 160 EAF, the Boudouard reaction, Eq. (3r), as well as the homogeneous and heterogeneous water-161 gas shift reactions, Eq. (3q) and (3s), are modeled. The reaction rates of these three reactions 162 are calculated with the corresponding equilibrium constant, which for simplification is assumed 163 to be only temperature-dependent and not composition-dependent. The molar reaction rate r164 can be determined by Eq. (4) while the equilibrium constant K_c is determined by the forward and backward reaction rate constant according to Eq. (5). The mole concentrations c_i are 165 166 obtained using Eq. (6) [15].

$$r = k_f \prod_{i=1}^{I} [c_i]^{v'_i} - k_b \prod_{i=1}^{I} [c_i]^{v''_i}$$
(4)

$$K_c = \frac{k_f}{k_b} \tag{5}$$

$$c_i = \frac{m_i}{M_i V_{gas}} \tag{6}$$

167 Here, v'_i and v''_i represent the stoichiometric coefficients of the forward (') and backward (") 168 reaction.

169 It is not possible to easily derive k_f and k_b from K_c or other data available to the model. Therefore, 170 to be able to solve the equation, the backward reaction rate constant is assumed to be $k_b = 1$, 171 leading to the simplified Eq. (7). In addition, in Eq. (10) an empirical velocity coefficient is 172 added.

$$r = K_c \prod_{i=1}^{l} [c_i]^{v'_i} - \prod_{i=1}^{l} [c_i]^{v''_i}$$
(7)

173 K_c can be determined by the idea of the free Gibbs energy minimization through Eq. (8) and 174 (9):

$$K_{p} = \exp\left(\frac{-\Delta_{R}G^{0}}{R_{m}T}\right) = \prod_{i} \left(\frac{p_{i}}{p^{0}}\right)_{e}^{v_{i}}$$

$$(8)$$

$$K_c = K_p \left(\frac{p^0}{R_m T}\right)^{\sum v_i} \tag{9}$$

175 where K_p is the standard equilibrium constant, $\Delta_R G^0$ represents the free standard enthalpy, p^0 is 176 the pressure at standard conditions, p_i the partial pressure and R_m the molar gas constant.

The equilibrium constant K_c is pre-calculated for each of the three equilibrium reactions with the help of the chemical equilibrium toolbox *MediumModel* [16] within Matlab, based on the "NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species" and stored in a temperature dependent database. The database is evaluated at each time step with a corresponding temperature to obtain the equilibrium constant $K_{c-(\zeta)}$ for the equilibrium reaction ($\xi = (q)$, (r) and (s)). The mass change for each element is then calculated using Eq. (10):

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = r_{(\xi)} v_i V_{(\xi)} M_i k d_{gas-(\xi)} \tag{10}$$

184 where $V_{(\xi)}$ is the available volume for the reaction and $kd_{gas-(\xi)}$ is an empirical velocity 185 coefficient. These velocity coefficients either were taken from Logar et al. [3] or were 186 developed during the parameterization of the modified model using the available operating data. 187 They are listed in Table 2 in the Appendix.

In contrast to the described equilibrium reactions above, the dissociation of H_2O , which is the reverse reaction of Eq. (3t), is modeled using a simplified empirical approach which is described later.

191 **2.3.2 Rate of Change of Carbon (C)**

Since carbon is involved in reactions within the gas phase, the equations of the carbon mass transfer were modified in comparison to those of Logar et al. [3]. In accordance with Logar and for a better overview, the mass flows of the respective elements *i* are divided based on their physical-chemical cause. These individual mass flows are denoted by the variable $x_{i_{dj}}$ (*j* = number for the individual mass flow). With their summation, the net mass flow of the element *i* (*m_i*) is determined.

The rate of change of carbon is calculated for three different masses of C in the EAF: First, the mass of C present in the EAF (m_{C-L}). Second, the dissolved C in the liquid melt (m_{C-D}) and third, the C from charge coal (m_{coal}).

The following mechanisms are relevant for the mass of C in the EAF (m_{C-L}): C is injected in the furnace (xI_{d1}). This injected C and the C present in the EAF is used in the decarburization of the melt (xI_{d2}). Furthermore, C is dissolved in the melt (xI_{d3}). C is formed during the dissociation of combustible material. This amount and the C from charged coal is available for further reactions (xI_{d4}). During the oxidation of C to CO with the oxygen of the gas phase (xI_{d5}) and with leak air (xI_{d6}), C is used. Finally, C is taking part in the heterogeneous water-gas reaction Eq. (3s) (xI_{d7}). The rate of change of C present in the EAF (\dot{m}_{C-L}) is given by Eq. (11):

$$\begin{aligned} x\mathbf{l}_{d1} &= \dot{m}_{C-inj} \\ x\mathbf{l}_{d2} &= \left(-\frac{kd_{C-L} m_{FeO} m_{C-L}^{0.75}}{m_{ISI}} - 0.6 \, x\mathbf{l}_{d1} \right) \left(1 - \frac{V_{sSc}}{V_{sSc,basket}} \right)^3 \\ x\mathbf{l}_{d2} &= \frac{kd_{C-3} m_{C-L}^{0.75} T_{ISc} C_{p,ISc} \frac{T_{air}}{T_{metr,Sc}}}{\lambda_c + C_{p,C} \left(T_{metr,Sc} - T_{air} \right)} \\ x\mathbf{l}_{d3} &= \frac{kd_{C-3} m_{C-L}^{0.75} T_{ISc} C_{p,ISc} \frac{T_{air}}{T_{metr,Sc}}}{M_{C9H20}} \\ x\mathbf{l}_{d4} &= -x\mathbf{l}coal_{d1} - \dot{m}_{comb} \frac{9M_{C}}{M_{C9H20}} \\ x\mathbf{l}_{d5} &= -K_{sSc-ISc}^4 kd_{C-5} m_{C-L}^{0.75} c_{O2-gas}^{0.5} \\ (11) \\ x\mathbf{l}_{d6} &= \begin{cases} 0 & , m_{C} < 1kg \\ -w_{O2-air} K_{leakair-O2-CO(1)} \dot{m}_{leakair} \frac{2M_{C}}{M_{O2}} , m_{C} > 1kg \\ x\mathbf{l}_{d7} &= -r_{(s)} V_{(s)} M_{C} kd_{gas-(s)} \\ \dot{m}_{C-L} &= \sum_{j=1}^{7} x\mathbf{l}_{dj} \end{cases} \end{aligned}$$

The equation for the variable xI_{d2} is an empirical equation, which was developed during the parameterization of the adapted model using the available operating data. kd_{C-L} is the constant decarburization velocity and m_{ISI} is the total slag mass. The second summand (0.6 xI_{d1}) represents a direct reaction of injected C with FeO. V_{sSc} is the actual bulk volume of the solid scrap and $V_{sSc,basket}$ the initial charged volume of sSc. The factor causes the chemical reaction in the simulation to start with increasing molten mass. If the furnace is full of scrap, the injected C does not reach the melt surface.

The equation for xI_{d3} is also an empirical equation, which resulted from the adaptation of Logar's equation during parameterization. The equation is dependent on the constant dissolving velocity kd_{C-3} , the temperatures of the melt T_{lSc} , of the ambient air T_{air} and the scrap's liquidus temperature $T_{melt,sSc}$, the heat capacities of C $C_{P,C}$ and the melt $C_{P,lSc}$ and the latent heat of fusion of C λ_C .

220 The combustible material consists of nonane and is denoted by \dot{m}_{comb} .

221 kd_{C-5} is the constant C oxidation velocity. $K_{sSc-lSc}$ is the exposure coefficient of the liquid bath,

because the reactionary surface of the melt decreases with increasing solid scrap volume. c_{O2} -

223 *gas* is the concentration of oxygen in the gas phase.

 w_{O2-air} is the mass fraction of O₂ in the ambient air, which is sucked in as leak air $\dot{m}_{leakair}$ through the slag door and other gaps. $K_{leakair-O2-CO(1)}$ is the fraction of leak air available for direct C combustion to CO. The equation is divided into two cases, because otherwise the simulation would lead to negative masses as calculation results.

The calculation of xI_{d5} and xI_{d6} are based on the empirical reaction kinetic approach according to Eq. (12) for the reaction given by Eq. (13):

$$-\frac{\mathrm{d}[c_{A}]}{\mathrm{d}t} = k[c_{A}]^{v_{A}}[c_{B}]^{v_{B}}$$
(12)

$$|v_A|A + |v_B|B \longrightarrow |v_C|C + |v_D|D$$
(13)

where *A* and *B* are reactants with the concentration c_A or c_B . The stoichiometric coefficients are signified with *v*, while *k* is the according reaction rate.

The calculation of the molar reaction rate $r_{(s)}$ in xI_{d7} follows the Eq. (14) and Eq. (15). The database for K_c is evaluated for the assumed average temperature between the gas phase and the liquid scrap. The reaction volume $V_{(s)}$ is determined for each equilibrium reaction ξ by Eq. (16) as a fraction of the total gas volume V_{gas} .

$$K_{c-(s)} = f\left(\frac{T_{gas} + T_{lSc}}{2}\right) \tag{14}$$

$$r_{(s)} = K_{c-(s)}c_{H2O}^{-1} - c_{CO}c_{H2}$$
(15)

$$V_{(\xi)} = x_{(\xi)} V_{gas} \tag{16}$$

Only in case of a negative relative furnace pressure p_r , the total mass flow of leak air enters the furnace. This is determined by Eq. (17) with K_{PR} representing a constant defining the ratio between mass flow and pressure:

$$\dot{m}_{leakair} = \begin{cases} 0 , p_r > 0 \\ K_{PR}p_r , p_r < 0 \end{cases}$$
(17)

The rate of change of <u>C from coal \dot{m}_{coal} </u> is determined by the following mechanisms: C is charged with coal within the scrap baskets. The reactive mass flow of C (*x1coal_{d1}*) is transferred from m_{coal} to m_{C-L} for decarburization, dissolving and combustion. Analogous to *x1_{d5}* and *x1_{d6}*,

- the amount of C from coal decreases due to the combustion of C to CO with the oxygen from
- 243 the gas phase $(x1coal_{d2})$ and from the leak air $(x1coal_{d3})$. C taking part in the Boudouard reaction
- Eq. (3r) ($x1coal_{d4}$). The mass change \dot{m}_{coal} is given by Eq. (18):

$$x1coal_{d1} = -kd_{C-4} m_{coal}^{0.75} \sqrt{1 - \frac{V_{sSc}}{V_{sSc,basket}}}$$

$$x1coal_{d2} = -kd_{C-6} m_{coal}^{0.75} c_{O2-gas}^{0.5}$$

$$x1coal_{d3} = \begin{cases} 0 & , m_{coal} < 1kg \\ -w_{air-O2} K_{leakair-O2-CO(2)} \dot{m}_{leakair} \frac{2M_{C}}{M_{O2}}, m_{coal} > 1kg \end{cases}$$

$$x1coal_{d4} = -r_{(r)} V_{(r)} M_{C} kd_{gas-(r)}$$

$$\dot{m}_{coal} = \sum_{j=1}^{4} x1coal_{dj}$$
(18)

 kd_{C-4} and kd_{C-6} represent the coal reactivity coefficients. The equations for $x1coal_{d1}$ and $x1coal_{d2}$ are developed empirical equations, which were validated by means of parametrization. The calculation of $r_{(r)}$ follows the Eq. (19) and Eq. (20), whereby the database for K_c is evaluated for the assumed average temperature.

$$K_{c-(r)} = f\left(\frac{T_{gas} + T_{lSc}}{2}\right)$$
(19)

$$r_{(r)} = K_{c-(r)}c_{CO2}^{-1} - c_{CO}^2$$
(20)

The rate of change of <u>dissolved C in the liquid melt (m_{C-D}) </u> is determined according to Logar's description with a few enhancements and is given by Eq. (21):

$$x2_{d1} = -kd_{C-D} \left(X_{C} - X_{C}^{eq} \right)$$

$$x2_{d2} = -kd_{C-1} \left(X_{C} - X_{C}^{eq} \right) \dot{m}_{02,lance} K_{02-CO} \frac{2M_{C}}{M_{02}}$$

$$x2_{d3} = -x1_{d3}$$

$$x2_{d4} = -kd_{Mn-1} \left(X_{MnO} - X_{MnO-1}^{eq} \right) \frac{M_{C}}{M_{MnO}}$$

$$x2_{d5} = -kd_{C-2} \left(X_{C} - X_{C}^{eq} \right) \dot{m}_{02-lance} K_{02-CO2} \frac{2M_{C}}{M_{02}}$$

$$\dot{m}_{C-D} = \sum_{j=1}^{5} x2_{dj}$$
(21)

where X_i and X_i^{eq} are the molar fractions and equilibrium molar fractions respectively, kd_{C-D} is the FeO decarburization rate, kd_{C-1} and kd_{C-2} are the oxidation rates of C to CO and CO₂ respectively, kd_{Mn-1} is the MnO decarburization rate and K_{O2-CO} and K_{O2-CO2} are representing the fractions of the lanced oxygen used for direct oxidization. The two change rates \dot{m}_{C-L} and \dot{m}_{C-D} can be further improved by the solution presented by Fathi et al. [5]. All other rates of change for the components of the steel and slag zone are not changed and are implemented according to Logar et al. [3].

258 **2.3.3 Rate of Change of Carbon Monoxide (CO)**

The rate of change of carbon monoxide in the gas phase (m_{CO}) is implemented by nine mechanisms: CO is extracted with the off-gas ($x9_{d1}$) and through openings ($x9_{d4}$). CO is produced during the incomplete oxidation of C from coal, injected carbon ($x9_{d2}$) and CH₄ ($x9_{d8}$). Furthermore, sources are electrode oxidation and the oxidation of coal ($x9_{d6}$). CO is consumed by the CO post-combustion ($x9_{d3}$) and changed due to the equilibrium reactions of the homogeneous water-gas shift reaction ($x9_{d5}$), the Boudouard reaction ($x9_{d7}$) and the heterogeneous water-gas reaction ($x9_{d9}$). The rate of change of CO is obtained by Eq. (22):

$$x9_{d1} = -\frac{h_{d}u_{1}m_{co}}{(k_{u}u_{2} + h_{d})m_{gas}}$$

$$x9_{d2} = -(x1_{d2} + x1_{d5} + x1_{d6} + x1coal_{d2} + x1coal_{d3} + x2_{d1} + x2_{d2} + x2_{d4})\frac{M_{co}}{M_{c}}$$

$$x9_{d3} = -kd_{co-1}m_{co}c_{02-gas}^{0.5} - \dot{m}_{02-post}K_{02-post-CO}\frac{2M_{co}}{M_{02}}$$

$$x9_{d4} = \begin{cases} -K_{PR}p_{r}\frac{m_{co}}{m_{gas}}, p_{r} > 0\\ 0, p_{r} < 0 \end{cases}$$

$$x9_{d5} = r_{(q)}V_{(q)}M_{co}kd_{gas-(q)}$$

$$x9_{d6} = -\dot{m}_{el}\frac{M_{co}}{M_{c}}$$

$$x9_{d8} = -(x15_{d5} + x15_{d8})\frac{M_{co}}{M_{CH4}}$$

$$(22)$$

$$x9_{d9} = -x1_{d7} \frac{M_{CO}}{M_C}$$
$$\dot{m}_{CO} = \sum_{j=1}^{9} x9_{dj}$$

The equation for $x9_{d1}$ is equal to Logar's [3] implementation with h_d being the characteristic dimension of the duct area at the slip gap, u_1 is the off-gas mass flow, k_U is a dimensionless constant and set to the same value as proposed by Bekker [17] and u_2 is the slip gap width.

 $269 \quad kd_{CO-1}$ is the reaction velocity of the CO post-combustion. In order to promote this reaction in

270 the EAF, an oxygen mass flow $\dot{m}_{O2-post}$ is injected via lance. Furthermore, $K_{O2-post-CO}$ is the

271 fraction of this post-combustion O₂ mass flow used for CO post-combustion.

The outflow of gas through openings is modeled analogously to the inflow of leak air in Eq. (16).

273 If an overpressure prevails in the vessel, furnace gas is discharged.

The reaction rate $r_{(q)}$ of $x9_{d5}$ is determined with the equilibrium constant $K_{c-(q)}$ by Eq. (23) and Eq. (24):

$$K_{c-(q)} = f\left(T_{gas}\right) \tag{23}$$

$$r_{(q)} = K_{c-(q)} c_{CO}^{-1} c_{H2O}^{-1} - c_{CO2} c_{H2}$$
(24)

276 $kd_{gas-(q)}$ is the reaction velocity of the homogeneous water-gas shift reaction and is – like all 277 other reaction velocities kd – given in Table 2 in the Appendix.

The graphite electrode oxidizes during the EAF operation. A minor mass of C (\dot{m}_{el}) releases, which can react with the gas phase. The corresponding calculation is described in Logar et al. [3].

281 **2.3.4 Rate of Change of Carbon Dioxide (CO₂)**

The rate of change of carbon dioxide in the gas phase (\dot{m}_{CO2}) is determined by the following mechanisms: CO₂ is extracted with the off-gas ($x10_{d1}$) and flows out through openings ($x10_{d7}$). CO₂ arises from CO post-combustion ($x10_{d2}$), CH₄ combustion ($x10_{d4}$ and $x10_{d6}$) and from dissolved C oxidation ($x10_{d8}$). CO₂ takes part in the equilibrium reactions of the homogeneous water-gas shift reaction $(x10_{d3})$ and the Boudouard reaction $(x10_{d5})$. The rate of change of CO₂

is obtained by Eq. (25):

$$x10_{d1} = -\frac{h_{d}u_{1}m_{co2}}{(k_{u}u_{2} + h_{d})m_{gas}}$$

$$x10_{d2} = -\frac{M_{co2}}{M_{co}}x9_{d3}$$

$$x10_{d3} = -x9_{d5}\frac{M_{co2}}{M_{co}}$$

$$x10_{d4} = -x15_{d4}\frac{M_{co2}}{M_{CH4}}$$

$$x10_{d5} = x1coal_{d4}\frac{M_{co2}}{M_{c}}$$

$$x10_{d6} = -x15_{d6}\frac{M_{co2}}{M_{CH4}}$$

$$x10_{d7} = \begin{cases} -K_{PR}p_{r}\frac{m_{co2}}{m_{gas}}, p_{r} > 0\\ 0 & , p_{r} < 0 \end{cases}$$

$$x10_{d8} = -x2_{d5}\frac{M_{co2}}{M_{c}}$$

$$\dot{m}_{co2} = \sum_{j=1}^{8}x10_{dj}$$

$$(25)$$

288 2.3.5 Rate of Change of Nitrogen (N₂)

The rate of change of nitrogen (m_{N2}) is determined by the extraction with the off-gas ($x11_{d1}$) and the outflow through openings ($x11_{d2}$ for $p_r > 0$). For a negative relative pressure, N₂ is sucked in with the leak air ($x11_{d2}$ for $p_r < 0$). Furthermore, N₂ is injected together with the injected O₂, CH₄ and C mass flows ($x11_{d3}$). Compared to Logar et al. [3], the rate of change of N₂ is supplemented by $x11_{d3}$ and determined by Eq. (26):

$$x 1 1_{d1} = -\frac{h_{d} u_{1} m_{N2}}{(k_{u} u_{2} + h_{d}) m_{gas}}$$

$$x 1 1_{d2} = \begin{cases} -K_{PR} p_{r} \frac{m_{CO}}{m_{gas}}, p_{r} > 0 \\ w_{N2-air} \dot{m}_{leakair}, p_{r} < 0 \end{cases}$$
(26)

$$x11_{d3} = \dot{m}_{CH\,4-inj} \frac{w_{N2-in-natgas}}{w_{CH\,4-in-natgas}} + \left(\dot{m}_{O2-lance} + \dot{m}_{O2-post} + \dot{m}_{O2-CH\,4-inj}\right) \frac{w_{N2-in-oxygen}}{w_{O2-in-oxygen}}$$
$$\dot{m}_{N2} = \sum_{j=1}^{3} x11_{dj}$$

where all w_i are the mass fractions of the following mass flows. w_{N2-air} is the mass fraction of N₂ in the leak air, $w_{N2-in-natgas}$ and $w_{CH4-in-natgas}$ are the mass fractions of N₂ and CH₄ in the injected natural gas respectively, $w_{N2-in-oxygen}$ and $w_{O2-in-oxygen}$ are the mass fractions of N₂ and O₂ in the injected oxygen mass flows. Therefore, the considered O₂ is injected via lance for the reduction of Fe ($\dot{m}_{O2-lance}$), via tuyere for post-combustion ($\dot{m}_{O2-post}$) and via the burner system ($\dot{m}_{O2-CH4-inj}$).

300 **2.3.6 Rate of Change of Oxygen (O2)**

301 The rate of change of oxygen in the gas zone (\dot{m}_{O2}) is determined by the following mechanisms: 302 O_2 is extracted with the off-gas $(x12_{d1})$ and flows out through openings in the EAF vessel $(x12_{d7})$ 303 for $p_r > 0$). For a negative relative pressure, O₂ is sucked in with leak air (x_{12d7} for $p_r < 0$). 304 Further, a residual O₂ mass flow remains of all O₂ lanced into the gas phase $(x12_{d2})$ due to 305 incomplete oxidation reactions, e.g. during the oxidation of dissolved C in the liquid melt ($x2_{d2}$ 306 and $x2_{d5}$), Si $(x3_{d2})$, Cr $(x5_{d2})$, P $(x6_{d2})$ and Fe $(x7_{d3})$. O₂ is injected with the natural gas though 307 the burner system into the EAF ($\dot{m}_{O2-CH4-inj}$), which reacts with CH₄ in different burner zones 308 $(x15_{di})$ and leaves a residual O₂ mass flow $(x12_{d3})$. O₂ is injected $(\dot{m}_{O2-post})$ for CO post-309 combustion $(x9_{d3})$ and leaves a residual mass flow $(x12_{d4})$. The oxidation of the electrodes 310 consumes O₂ ($x12_{d5}$) as well as the combustion of coal and C in the EAF ($x12_{d6}$). In addition 311 the post-combustion of CH₄ ($x12_{d8}$) also uses up O₂. The post-combustion of H₂ ($x13_{d4}$) is 312 combined with the dissociation of H₂O ($x14_{d5}$) in the change of O₂ ($x12_{d9}$). The total rate of 313 change of O_2 is determined with Eq. (27):

$$x12_{d1} = -\frac{h_d u_1 m_{O2}}{\left(k_u u_2 + h_d\right) m_{gas}}$$
(27)

$$\begin{aligned} x 12_{d2} &= \dot{m}_{02-lance} + x2_{d2} \frac{M_{02}}{2M_c} + x2_{d3} \frac{M_{02}}{M_c} + x3_{d2} \frac{M_{02}}{M_{si}} + x5_{d2} \frac{3M_{02}}{4M_{cr}} + x6_{d2} \frac{5M_{02}}{4M_p} - x7_{d3} \frac{M_{02}}{2M_{FeO}} \\ x 12_{d3} &= \dot{m}_{02-CH4-inj} + x15_{d4} \frac{2M_{02}}{M_{CH4}} + x15_{d5} \frac{3M_{02}}{2M_{CH4}} + x15_{d6} \frac{M_{02}}{M_{CH4}} \\ x 12_{d4} &= \dot{m}_{02-post} + x9_{d3} \frac{M_{02}}{2M_{cO}} \\ x 12_{d5} &= \dot{m}_{el} \frac{M_{02}}{2M_c} \\ x 12_{d6} &= (x1_{d5} + x1_{d6} + x1coal_{d2} + x1coal_{d3}) \frac{M_{02}}{2M_c} \\ x 12_{d7} &= \begin{cases} -K_{PR} p_r \frac{m_{02}}{m_{gas}}, p_r > 0 \\ w_{air-02} \dot{m}_{leakair}, p_r < 0 \end{cases} \\ x 12_{d9} &= x13_{d4} \frac{M_{02}}{2M_{H2}} - x14_{d5} \frac{M_{02}}{2M_{H2O}} \\ x 12_{d9} &= \sum_{j=1}^{9} x12_{dj} \end{aligned}$$

314 **2.3.7 Rate of Change of Hydrogen (H₂)**

The rate of change of hydrogen in the gas zone (\dot{m}_{H2}) is determined by the following mechanisms: H₂ is extracted with the off-gas $(x13_{d1})$ and flows out through openings $(x13_{d2})$. There is an assumed H₂ residual mass flow caused by an incomplete CH₄ combustion from burners $(x13_{d3})$. H₂ is produced during the dissociation of combustible materials $(x13_{d7})$ and H₂ is consumed during post-combustion $(x13_{d4})$. Furthermore, H₂ takes part in the equilibrium reactions of the heterogeneous $(x13_{d5})$ and homogeneous water-gas reactions $(x13_{d6})$. The rate of change is obtained by Eq. (28):

$$x13_{d1} = -\frac{h_{d}u_{1}m_{H2}}{(k_{u}u_{2} + h_{d})m_{gas}}$$

$$x13_{d2} = \begin{cases} -K_{PR}p_{r}\frac{m_{H2}}{m_{gas}}, p_{r} > 0\\ 0, p_{r} < 0 \end{cases}$$

$$x13_{d3} = -x15_{d6}\frac{2M_{H2}}{M_{CH4}}$$
(28)

$$x13_{d4} = -kd_{H2-post}m_{H2}c_{O2-gas}^{0.5}$$

$$x13_{d5} = -x1_{d7}\frac{M_{H2}}{M_{C}}$$

$$x13_{d6} = -x9_{d5}\frac{M_{H2}}{M_{C0}}$$

$$x13_{d7} = -\dot{m}_{comb}\frac{10M_{H2}}{M_{C9H20}}$$

$$\dot{m}_{H2} = \sum_{j=1}^{7}x13_{dj}$$

322 where $kd_{H2-post}$ is the reaction rate constant of the H_2 post-combustion.

323 **2.3.8 Rate of Change of Water Vapour (H2O)**

324 The rate of change of water vapour in the gas zone (\dot{m}_{H2O}) is determined by the following mechanisms: H₂O is extracted with the off-gas $(x14_{d1})$ and flows out through openings $(x14_{d2})$ 325 326 and enters the EAF via the electrode cooling $(x14_{d3})$. To decrease the electrode consumption, 327 the graphite electrode is equipped with a water spray cooling system at its top. The water (\dot{m}_{water} -328 in) flows down the electrode and evaporates, whereby a part of the steam is assumed to enter 329 the EAF vessel. Furthermore, H₂O is a product of the CH₄ ($x14_{d4}$ and $x14_{d6}$) and H₂ combustion 330 $(x14_{d7})$. H₂O takes part in the equilibrium reactions of the heterogeneous $(x14_{d8})$ and 331 homogeneous water-gas reactions ($x_{14_{d9}}$). $x_{14_{d5}}$ describes a simplified exponential approach 332 for the dissociation of water, as the dissociation is encouraged by attendance of metal oxides 333 [18]. The rate of change is obtained by Eq. (29):

$$x 14_{d1} = -\frac{h_{d}u_{1}m_{H2O}}{(k_{u}u_{2} + h_{d})m_{gas}}$$

$$x 14_{d2} = \begin{cases} -K_{PR}p_{r}\frac{m_{H2O}}{m_{gas}}, p_{r} > 0\\ 0, p_{r} < 0 \end{cases}$$

$$x 14_{d3} = -\dot{m}_{water-in}$$

$$x 14_{d4} = -x 15_{d8}\frac{2M_{H2O}}{M_{CH4}}$$

$$x 14_{d5} = -kd_{H2O}\exp\left(\frac{m_{H2O}}{5}\right)$$

$$x 14_{d6} = -(x 15_{d4} + x 15_{d5})\frac{2M_{H2O}}{M_{CH4}}$$
(29)

$$x14_{d7} = -x13_{d4} \frac{M_{H2O}}{M_{H2}}$$
$$x14_{d8} = x1_{d7} \frac{M_{H2O}}{M_C}$$
$$x14_{d9} = -x9_{d5} \frac{M_{H2O}}{M_{CO}}$$
$$\dot{m}_{H2O} = \sum_{j=1}^{9} x14_{dj}$$

334 **2.3.9 Rate of Change of Methane (CH4)**

The rate of change of methane in the gas zone (\dot{m}_{CH4}) is determined by the following mechanisms: CH₄ is extracted with the off-gas ($x15_{d1}$) and flows out through openings ($x15_{d2}$). Natural gas, which consists mainly of CH₄, is injected through the burner system ($x15_{d3}$). The CH₄ is assumed to react in three different ways ($x15_{d4}$, $x15_{d5}$ and $x15_{d6}$) and finally, CH₄ is postcombusted ($x15_{d7}$). The rate of change is obtained by Eq. (30):

$$x15_{d1} = -\frac{h_{d}u_{1}m_{CH4}}{(k_{u}u_{2} + h_{d})m_{gas}}$$

$$x15_{d2} = \begin{cases} -K_{PR}p_{r}\frac{m_{CH4}}{m_{gas}}, p_{r} > 0\\ 0, p_{r} < 0 \end{cases}$$

$$x15_{d3} = \dot{m}_{CH4-inj}$$

$$x15_{d4} = \begin{cases} -K_{burn-(n1)}x15_{d3}, Z \le Z_{St-(n1)}\\ -K_{O2-CH4-inj}K_{burn-(n1)}\dot{m}_{O2-CH4-inj}\frac{M_{CH4}}{2M_{O2}}, Z > Z_{St-(n1)}\\ -K_{O2-CH4-inj}K_{burn-(n2)}\dot{m}_{O2-CH4-inj}\frac{2M_{CH4}}{3M_{O2}}, Z > Z_{St-(n2)}\\ -K_{O2-CH4-inj}K_{burn-(n2)}\dot{m}_{O2-CH4-inj}\frac{2M_{CH4}}{3M_{O2}}, Z > Z_{St-(n2)}\\ -K_{O2-CH4-inj}K_{burn-(n2)}\dot{m}_{O2-CH4-inj}\frac{M_{CH4}}{3M_{O2}}, Z > Z_{St-(n2)}\\ x15_{d5} = \begin{cases} -K_{burn-(n3)}x15_{d3}, Z \le Z_{St-(n3)}\\ -K_{O2-CH4-inj}K_{burn-(n3)}\dot{m}_{O2-CH4-inj}\frac{M_{CH4}}{M_{O2}}, Z > Z_{St-(n3)}\\ -K_{O2-CH4-inj}K_{burn-(n3)}\dot{m}_{O2-CH4-inj}\frac{M_{CH4}}{M_{O2}}, Z > Z_{St-(n3)}\\ x15_{d7} = -kd_{CH4-post}m_{CH4}c_{O2-gas}^{1.5}\\ \dot{m}_{CH4} = \sum_{j=1}^{7}x15_{dj} \end{cases}$$
(30)

340 where $kd_{CH4-post}$ represents the reaction rate of CH₄ post-combustion. It is assumed that there 341 are three different reaction zones of the burner flame due to the non-premixed supply of CH₄ and O₂. Within the reaction volumes, the respective reactions of Eq. $(6n_1)$, $(6n_2)$ and $(6n_3)$ take place. Therefore, $K_{burn-(n1)}$, $K_{burn-(n2)}$ and $K_{burn-(n3)}$ are the corresponding percentages of the reaction volumes.

The reaction rates are limited by the ratio of O_2 to CH_4 . The stoichiometric mixture fraction Z_{St} . (*ni*) according to Peters [19] is compared with the actual mixture fraction Z of the supplied gas mass flows, which is defined according to Eq. (31):

$$Z = \frac{\dot{m}_{CH4-inj}}{\dot{m}_{CH4-ini} + \dot{m}_{02-CH4-ini}}$$
(31)

348 The stoichiometric mixing fraction $Z_{St-(ni)}$ is obtained in general by Eq. (32) and for the three 349 reactions according to Eq. (33) to (35):

$$Z_{St-(ni)} = \frac{v_{CH4,i} M_{CH4}}{v_{CH4,i} M_{CH4} + v_{02,i} M_{02} \frac{W_{CH4-in-natgas}}{W_{02-in-oxygen}}}$$
(32)

$$Z_{St-(n1)} = \frac{M_{CH4}}{M_{CH4} + 2M_{O2}} \frac{W_{CH4-in-natgas}}{W_{O2-in-oxygen}}$$
(33)

$$Z_{St-(n2)} = \frac{M_{CH4}}{M_{CH4} + \frac{3}{2}M_{O2}\frac{W_{CH4-in-natgas}}{W_{O2-in-oxygen}}}$$
(34)

$$Z_{St-(n3)} = \frac{M_{CH4}}{M_{CH4} + M_{O2}} \frac{W_{CH4-in-natgas}}{W_{O2-in-natgas}}$$
(35)

For $Z \le Z_{St}$, the natural gas mass flow $x15_{d3}$ is completely consumed and for $Z > Z_{St}$ the reaction rate is limited by the available fraction of the burner oxygen. $K_{O2-CH4-inj}$ is the fraction of the injected O₂ mass flow available for direct CH₄ combustion. This empirical factor is calculated according to the coverage of the burner nozzle openings by scrap (e.g. after scrap charging). In this case, only an insufficient mixing of the two gases CH₄ and O₂ is assumed, which leads to an incomplete reaction of CH₄. $K_{O2-CH4-inj}$ is calculated with Eq. (36), which has been empirically derived based on the scrap meltdown progress in front of the burner nozzle:

$$K_{O2-CH4-inj} = 1 - 0.75 \left(\frac{m_{sSc}}{m_{sSc,basket}}\right)^2$$
(36)

357 where $m_{sSc,basket}$ represents the mass of scrap charged into the EAF.

Together with the scrap, combustible materials like grease, oils and paints enter into the EAF. These materials are taken into account as a mass of Nonan (C_9H_{20}) and it is assumed, that C_9H_{20} dissociates before further reactions take place. The dissociation follows the empirical approach in Eq. (37), which has been adopted from Logar et al. [3] and adjusted to improve the agreement of simulation and measurement results.

$$\dot{m}_{comb} = -kd_{comb}m_{comb}^{0.75} \left(1.1 - \frac{V_{sSc}}{V_{sSc,basket}}\right)^2$$
(37)

363 **2.4. Reaction Enthalpies**

Chemical reactions lead to a conversion of energy. Exothermic or endothermic reactions are releasing or consuming energy to the corresponding zone or phase in which the reaction takes place. The enthalpy of the reactions is therefore computed according to Logar et al. [3] by Eq. (38):

$$\Delta H_{T}^{0} = \sum \Delta H_{298}^{0} (products) - \sum \Delta H_{298}^{0} (reactants) + \int_{298 K}^{T} \left[\sum C_{P} (products) - \sum C_{P} (reactants) \right] dT$$
(38)

with ΔH_{298}^{0} being the standard enthalpy of formation at standard temperature and pressure. By using the actual variables and reaction indices presented in Eq. (3) and by Logar et al. [3], the change of enthalpy is obtained for the implemented reactions according to Eq. (38) to (49) in **Table 1**.

372 Compared to Logar [3], the enthalpy of the reaction of the combustibles C_9H_{20} is calculated 373 according to the dissociation reaction in Eq. (3p), where C_9H_{20} and C are assumed with standard 374 temperature. All other reaction enthalpies $\Delta H^{0}_{T-(a)}$ to $\Delta H^{0}_{T-(m)}$ are implemented according to 375 Logar et al. [3] with adaptions in the equations for $\Delta H^{0}_{T-(g)}$ and $\Delta H^{0}_{T-(h)}$. The energy of the chemical reactions are allocated to the heat balance of the corresponding zones lSc and gas via the heats $Q_{lSc-chem}$ and $Q_{gas-chem}$ according to Eq. (50) and (51):

$$Q_{lSc-chem} = \sum_{\text{var}_{i}=(a)}^{(m)} \Delta H^{0}_{T-(\text{var}_{i})} - \Delta H^{0}_{T-(h)}$$
(50)

$$Q_{gas-chem} = \sum_{\text{var}_{i}=(n)}^{(u)} \Delta H^{0}_{T-(\text{var}_{i})} + \Delta H^{0}_{T-(h)}$$
(51)

378 where $Q_{gas-chem}$ is a further summand in the balance of Q_{gas} , which is implemented according to 379 Logar et al. [2].

380 3. Results and Discussion

381 This section present the simulation results, which are relevant for the modeling and simulation 382 of the EAF off-gas. The results are compared to measured data from an industrial scale EAF 383 with a tapping weight of approximately 140 t. The process simulation was performed with 384 MATLAB R2015b on a PC with 3.4 GHz, 16 GB RAM and Windows 7 64 bit. The relative 385 integration tolerance was set to 10^{-9} . For the simulation, the input data for scrap and operational 386 data for power and mass flows into the EAF were used while the hot heel was assumed constant 387 with a mass of 30 t. The operational data used has a resolution of five seconds and was evaluated 388 with an interpolation approach for each integration time step to determine the input mass flows 389 and powers. In total, 126 heats were simulated and evaluated in terms of energy and mass 390 balance. Furthermore, the steel, slag and gas compositions and temperatures were compared.

In the following, the results from single heats are compared as well as averaged results from all
126 heats. Thereby, transient behavior that cannot be reproduced by the simulation is smoothed
over and leads to a better comparability of the results.

Figure 2 shows the measured (meas) and simulated (sim) mass fractions of CO in black and CO₂ in grey as parts of the gas phase for a single heat. The charging of the second scrap basket is obvious at 20% relative time. The curves for CO are in the same range of magnitude with the biggest differences of 20% occurring at approximately 38% and 50% relative process time. For CO₂, the mass fractions are in the same range of magnitude during the melting of the first scrap 399 basket. During the melting of the second scrap basket and the refining phase, the simulated 400 mass fraction is about 8% higher than the measured fraction. In this case, the post combustion, 401 carbon reactions in the EAF and the equilibrium reactions need further adjustment but the 402 results are already satisfactory. Further conclusions can be drawn by analyzing the mass 403 fractions of H₂ and H₂O.



404

405 **Fig. 2.** Measured (meas) and simulated (sim) mass fractions w_i of CO and CO₂ in the off-gas 406 of a single heat

407 Therefore, **Figure 3** shows their mass fractions, as these components were added to the gas 408 phase simulation and are relevant for the equilibrium reactions. These components occur in 409 small amounts compared to CO and CO₂, so that the scale of the y-axis has to be adjusted 410 accordingly. The course of the measured and simulated mass fractions are in the same range of 411 magnitude with a bigger difference in H_2 at 40% process time, which can be associated with 412 non-stationary behavior of the melting.

413 For a further comparison of the results with less influence of instationarities, the averaged mass

414 fractions of CO and CO₂ for 126 heats are presented in Figure 4. It is obvious, that the

415 simulated fraction of CO is approximately 10% higher than the measured fraction after charging

416 the second scrap basket. In contrast, the simulated CO fraction is below the measured fraction

417 during the refining phase. The conversion of CO in the EAF through combustion and 418 decarburization needs to be shifted further to the refining. In case of CO₂, the simulated 419 fractions are close to the measured values.



421 **Fig. 3.** Measured (meas) and simulated (sim) mass fractions w_i of H_2 and H_2O in the off-gas 422 of a single heat



423

420

424 **Fig. 4.** Averaged measured (meas) and simulated (sim) mass fractions w_i of CO and CO₂ in 425 the off-gas for 126 heats

426 The averaged mass fractions of H_2 and H_2O are presented in **Figure 5**. For H_2O , the simulation

427 results are higher than the measured values at 10% and 30% process time. Here, the natural gas

428 injection is at a maximum and more water vapour is created through CH₄ combustion in the
429 simulation than in the real process. Further adjustment of the CH₄ reactions is necessary, but
430 the results are already satisfactory.





Fig. 5. Averaged measured (meas) and simulated (sim) mass fractions w_i of H₂ and H₂O in
 the off-gas for 126 heats

434 The chemical reactions in the gas phase have an influence on the gas temperature, which is 435 shown in **Figure 6** for a single heat and averaged for all simulated heats in **Figure 7**. While the 436 simulated temperature curve for a single heat shows a satisfactory result, the average 437 temperature shows bigger deviations of the simulated off-gas temperature. Especially during 438 the melting of the second scrap basket and the refining phase, the simulated temperature is always higher than the measured temperature. To investigate the influence of the temperature 439 440 on the total energy balance of the EAF, the specific off-gas enthalpy of all 126 heats is given in 441 Figure 8 as boxplots. The off-gas temperature difference is visible in the higher sensible 442 enthalpy output for the simulation. Compared to the latent enthalpy with medians at 140 kWh t⁻ ¹, which is the chemical energy of CO, H_2 and CH₄, the sensible enthalpy with medians at 443 around 50 kWh t⁻¹ is lower. The difference of the simulated off-gas temperature has less 444

445 influence on the off-gas energy output than a difference in the simulated off-gas composition



446 compared to the real process.

447





450 Fig. 7. Averaged measured (meas) and simulated (sim) off-gas temperature for 126 heats





452 **Fig. 8.** Boxplots of the measured and simulated off-gas enthalpy of 126 heats

Finally, the averaged mass flows of CO for the newly implemented chemical equilibrium reactions are shown in **Figure 9**. During the whole process, the equilibrium reactions lead to a production of CO. The amounts of up to 0.7 kg s⁻¹ demonstrate the relevance of considering these reactions in the gas phase modeling.



457

458 **Fig. 9.** Averaged CO mass flows of the equilibrium reactions from Boudouard $(x9_{d7})$, the 459 heterogeneous water-gas reaction $(x9_{d9})$ and the homogeneous water-gas reaction $(x9_{d5})$

460 It can be seen, that the consideration of further gas components and equilibrium reactions in the

461 gas phase lead to a better gas phase simulation in a dynamic process simulation model of an

462 EAF. This is important, as the off-gas temperature and composition are continuously463 measurable process values and represent one of the biggest energy outputs of the EAF.

Finally, the duration of the simulation is important for the applicability of the dynamic process
model. The further enhancement of the model leads to a higher complexity while the ODEsolver accelerates the simulation. For a single heat, the simulation time is between 65 s and 85 s.
Due to the ability of parallel computing, the 126 heats are simulated on four processor cores in
less than one hour. That means that the model is applicable for online process optimization.

469 **4. Conclusion**

In this paper, the enhancement of the gas phase of the dynamic EAF process model by Logar et al. [2, 3] is presented. The gas components H₂, H₂O and CH₄ were included in the gas phase modeling. These components were integrated into the calculation of chemical reactions under consideration of the equilibrium reactions of Boudouard and the water-gas reaction. To prevent the increase of simulation time due to the higher complexity, the model was re-implemented in MATLAB to use the more efficient ODE-solver ode15s for stiff ODE-systems.

476 The presented results of the enhanced EAF model were compared to measured data from an 477 industrial scale EAF. The off-gas mass fractions for single heats as well as averaged data show 478 a satisfactory similarity. The simulation of the gas phase temperature shows bigger differences, 479 which have a negligible influence on the simulated off-gas energy output. The implemented 480 equilibrium reactions show their significance on the CO production in the EAF. Further 481 optimization is still necessary. Especially the conversion of C through combustion and 482 decarburization has to be improved. Therefore, further measurements and data is necessary, 483 especially concerning the slag mass and mass of the hot heel. In the future, the model has to 484 prove its applicability for different EAFs and thereby the extrapolation capability for offline 485 investigations.

486 The simulation results were obtained in about one minute for each heat, so that the model is 487 applicable for online optimization. In addition, the parallel computing allows the simulation of

29

hundreds of different settings, input materials or operation strategies within a reasonable time.
With that, the model is appropriate for operator training and offline investigations on input
materials and modes of operation to reduce costs and energy consumption and increase the
energy and resource efficiency.

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527	Appendices			
528	List of symbols			
529	Greek letters			
530	λ	Latent heat of fusion		
531	v	Stoichiometric coefficient		
532	<i>v'</i>	Stoichiometric coefficient of the forward reaction		
533	<i>v''</i>	Stoichiometric coefficient of the backward reaction		
534	ρ	Density		
535	Latin letters			
536	ΔH_T^0	Reaction enthalpy at temperature T and standard pressure p^0		
537 538	ΔH^0_{298}	Standard formation enthalpy at standard temperature (298 K) and standard pressure p^0		
539	$\Delta H_{T-()}^0$	Standard formation enthalpy at T and standard pressure p^0 for a specific		
540		reaction		
541	$\Delta_R G^0$	Free standard enthalpy		
542	Α	Reacting element of the reaction $ v_A A + v_B B \longrightarrow v_C C + v_D D$		
543	В	Reacting element of the reaction $ v_A A + v_B B \longrightarrow v_C C + v_D D$		
544	С	Concentration		
545	С	Reagent of the reaction $ v_A A + v_B B \longrightarrow v_C C + v_D D$		
546	C_p	Heat capacity		
547	D	Reagent of the reaction $ v_A A + v_B B \longrightarrow v_C C + v_D D$		
548	h_d	Characteristic dimension of duct are at the slip gap		
549	k	Reaction rate constant		
550	k_b	Backward reaction rate constant		
551	k_{f}	Forward reaction rate constant		
552	<i>k</i> _u	Dimensionless constant		
553	kd	Empirical velocity coefficient		
554	kd _{C-1}	Empirical velocity coefficient for oxidation of dissolved C with injected O_2 to		
555		СО		
556	kd_{C-2}	Empirical velocity coefficient for oxidation of dissolved C with injected O_2 to		
557		CO_2		

Empirical velocity coefficient for dissolving of injected C 32

558

kdс-з

559	kd_{C-4}	Empirical velocity coefficient for dissolving of C from charged coal
560	kd_{C-5}	Empirical velocity coefficient for oxidation of injected C with O_2 from gas
561		phase to CO
562	kd _{C-6}	Empirical velocity coefficient for oxidation of C from charged coal with O_2
563		from gas phase to CO
564	kd _{C-D}	Empirical velocity coefficient for dissolving C in melt
565	kd _{C-L}	Empirical velocity coefficient for decarburization
566	kdco-1	Empirical velocity coefficient for oxidation of CO with O_2 from the gas phase
567		to CO ₂
568	kd _{CH4-post}	Empirical velocity coefficient for oxidation of CH_4 with O_2 from the gas phase
569	<i>kd</i> _{comb}	Empirical velocity coefficient for the oxidation of combustible material
570	kd _{gas-(ξ)}	Empirical velocity coefficient of equilibrium reaction in gas phase ($\xi = (q)$, (r),
571		(s))
572	kd _{H2-post}	Empirical velocity coefficient for oxidation of H_2 with O_2 from the gas phase
573		to H ₂ O
574	kd _{H2O}	Empirical velocity coefficient for the dissociation of water
575	kd _{Mn-1}	Empirical velocity coefficient for MnO decarburization
576	Κ	Fractions of mass, which is available for a specific reaction
577	$K_{burn-(n)}$	Fraction of the burner reaction volume for the reaction $(n1)$, $(n2)$ or $(n3)$
578	$K_{leakair-O2-CO(1)}$	Fraction of O_2 , sucked in with leak air, available for the oxidation of injected
579		C to CO
580	$K_{leakair-O2-CO(2)}$	Fraction of oxygen, sucked in with leak air, available for the oxidation of C
581		from charged coal to CO
582	$K_{O2\text{-}CH4\text{-}inj}$	Fraction of O_2 injected with CH_4 from burners available for the direct
583	(combustion of CH ₄
584	Ко2-со	Fraction of injected O ₂ available for the oxidation of dissolved C to CO
585	<i>K</i> _{02-C02}	Fraction of injected O_2 available for the oxidation of dissolved C to CO_2
586	K _{02-post-C0}	Fraction of injected O_2 available for the oxidation of CO to CO_2
587	$K_c \text{ or } K_{c-(\xi)}$	Equilibrium constant ($\xi = (q), (r), (s)$)
588	K_p	Standard equilibrium constant
589	<i>K</i> _{PR}	Constant defining the ration between mass flow and pressure
590	$K_{sSc-lSc}$	Correction factor, which includes the influence of solid scrap on the size of the
591		reaction surface of lSc
592	m	Mass

593	'n	Mass flow
594	\dot{m}_{el}	Mass flow of C released from electrode consumption
595	<i>ṁ</i> water-in	Mass flow of water from electrode cooling
596	İİ solidify	Mass flow from liquid to solid scrap if solidification occurs
597	М	Molar mass
598	р	Pressure
599	p^0	Pressure at standard conditions
600	p_i	Partial pressure of element <i>i</i>
601	<i>p</i> _r	Relative pressure in EAF
602	Р	Power
603	$Q_{lSc\text{-}chem}$	Heat from chemical reactions in melt
604	$Q_{\it gas-chem}$	Heat from chemical reaction in gas phase
605	Ż	Heat flow
606	r	Molar reaction rate
607	<i>Γ</i> (ξ)	Molar reaction rate ($\xi = (q), (r), (s)$)
608	R_m	Molar gas constant
609	t	Time
610	t_{tap}	Tap Time
611	Т	Temperature
612	<i>U</i> ₁	Off-gas mass flow
613	u_2	Slip gap width
614	V	Volume
615	$V_{(\xi)}$	Reaction volume of equilibrium reaction ($\xi = (q), (r), (s)$)
616	W	Weight fraction
617	$\chi_{(\zeta)}$	Fraction of reaction volume of equilibrium reaction in the gas phase volume
618	xi	Mass flow of element <i>i</i>
619	X_i	Molar fraction of element <i>i</i>
620	X_i^{eq}	Equilibrium molar fraction of element i in a specific reaction
621	Ζ	Actual mixing fraction of the supplied gas volume flows
622	$Z_{St-(n)}$	Stoichiometric mixing fraction of the reaction (n1), (n2) or (n3)
623		
624	List of subscr	ipts
625	Greek letters	
626	ξ	Equilibrium reaction ($\xi = (q), (r), (s)$)

627	Latin letters	
628	air	Ambient Air
629	addition	Added to a phase xx
630	b	Backward
631	C-inj	With lances injected carbon
632	C-D	Carbon dissolved in melt
633	C-L	Carbon present in EAF
634	C-S	Solid carbon
635	CH4-inj	Injected methane from burners
636	CH4-in-natgas	Methane in injected natural gas mass flow in burners
637	coal	Charged coal
638	f	Forward
639	gas	Gas phase in the EAF
640	H2O-gas	Gaseous water
641	i	Element ($i = 1$: C in EAF; $i = 1$ coal: C from charged coal; $i = 2$: dissolved C;
642		i = 9: CO; $i = 10$: CO ₂ ; $i = 11$: N ₂ ; $i = 12$: O ₂ etc.)
643	j	Number of individual mass flow (xi_{dj})
644	i,meas	Measured value of property of element <i>i</i>
645	i,sim	Simulated value of property of element <i>i</i>
646	leakair	Leak air
647	lSc	Liquid scrap phase in EAF
648	lSl	Liquid slag phase in EAF
649	melt,sSc	Melting point of solid scrap
650	N2-air	Nitrogen in ambient air
651	N2-in-natgas	Nitrogen in injected natural gas mass flow in burners
652	N2-in-oxgen	Nitrogen in injected O ₂ mass flow
653	O2-air	Oxygen in ambient air
654	O2-CH4-inj	Oxygen injected with CH ₄ in burners
655	O2-gas	Oxygen in gas phase
656	O2,lance	With lances injected oxygen
657	02-in-oxgen	Oxygen in injected O ₂ mass flow
658	O2-post	Oxygen injected for post-combustion
659	sSc	Solid scrap phase in EAF
660	sSc,basket	Solid scrap charged with basket

661	xx	Phase (sSc, lSc, sSl, lSl, gas, wall, el, arc)
662		
663	Abbreviations	
664	BDF	Backward differentiation formula
665	comb	Combustible material
666	EAF	Electric arc furnace
667	el	Electrode
668	lSc	Liquid scrap
669	1S1	Liquid slag
670	meas	Measured
671	NDF	Numerical differentiation formula
672	ODE	Ordinary differential equations
673	sim	Simulated
674	sSc	Solid scrap
675	sSl	Solid slag
676	St	Stoichiometric
677		

Table 2 gives the reaction rates kd used in the model. In Table 3 all necessary fractions (weight fractions w, fraction constants K for the reactions and volume fractions x for the reaction volumes) are listed. Table 4 contains all other constant parameters used in the model. Table 5, the used values of thermodynamical and physical constants (e.g. molar masses M_i and heat capacities $C_{p,i}$) are listed.

- 683 All values are adopted from Logar et al. [2, 3], partially adapted and/or supplemented. The
- values were validated and parameterized by using industrial furnace data.

685 Tables

686	Table 1.	Enthalpy reactions.	
	reaction according to Eq. (3) or Logar et al. [3]	Implemented formula for the enthalpy of the according reaction	Eq.
	(g)	$\Delta H_{T-(g)}^{0} = \frac{x 1_{d5} + x 1_{d6} + x 1_{coal_{d2}} + x 1_{coal_{d3}} + x 2_{d2}}{M_{c}}$ $\left[\left(\Delta H_{co}^{0} - \Delta H_{c-s}^{0} \right) + \int_{298K}^{T} \left(C_{p,co} - C_{p,c} - \frac{1}{2} C_{p,o2} \right) dT \right]$	(38)
	(h)	$\Delta H_{T-(h)}^{0} = \frac{x 9_{d3}}{M_{co}} \left[\left(\Delta H_{co2}^{0} - \Delta H_{co}^{0} \right) + \int_{298K}^{T} \left(C_{p,co2} - C_{p,co} - \frac{1}{2} C_{p,o2} \right) dT \right]$	(39)
	(n)	$\begin{split} \Delta H_{T-(n)}^{0} &= \frac{x15_{d4}}{M_{CH4}} \Bigg[\left(\Delta H_{CO2}^{0} + \Delta H_{H2O}^{0} - \Delta H_{CH4}^{0} \right) \\ &+ \int_{298K}^{T} \left(C_{p,CO2} + 2C_{p,H2O-g} - C_{p,CH4} - 2C_{p,O2} \right) dT \Bigg] \\ &+ \frac{x15_{d5} + x15_{d8}}{M_{CH4}} \Bigg[\left(\Delta H_{CO}^{0} + 2\Delta H_{H2O}^{0} - \Delta H_{CH4}^{0} \right) \\ &+ \int_{298K}^{T} \left(C_{p,CO} + 2C_{p,H2O-g} - C_{p,CH4} - \frac{3}{2}C_{p,O2} \right) dT \Bigg] \\ &+ \frac{x15_{d6}}{M_{CH4}} \Bigg[\left(\Delta H_{CO2}^{0} - \Delta H_{CH4}^{0} \right) \\ &+ \int_{298K}^{T} \left(C_{p,CO2} + 2C_{p,H2} - C_{p,CH4} - C_{p,O2} \right) dT \Bigg] \end{split}$	(40)
	(p)	$\Delta H^{0}_{T-(p)} = \frac{\dot{m}_{comb}}{M_{C9H20}} \left[\left(9 \Delta H^{0}_{C-S} - \Delta H^{0}_{C9H20} \right) + \int_{298K}^{T} C_{p,H2} dT \right]$	(44)

(q)

$$\Delta H_{T-(q)}^{0} = \frac{x9_{d5}}{M_{CO}} \left[\left(\Delta H_{CO2}^{0} - \Delta H_{CO}^{0} - \Delta H_{H2O}^{0} \right) + \int_{298K}^{T} \left(C_{p,CO2} + C_{p,H2} - C_{p,CO} - C_{p,H2O} \right) dT \right]$$
(45)

(r)

$$\Delta H_{T-(r)}^{0} = \frac{x 10_{d5}}{M_{CO2}} \left[\left(2 \Delta H_{CO}^{0} - \Delta H_{C-S}^{0} - \Delta H_{CO2}^{0} \right) + \int_{298K}^{T} \left(2 C_{p,CO} - C_{p,C} - C_{p,CO2} \right) dT \right]$$
(46)

(s)

$$\Delta H_{T-(s)}^{0} = \frac{x 1 4_{d8}}{M_{H20}} \left[\left(\Delta H_{C0}^{0} - \Delta H_{C-S}^{0} - \Delta H_{H20}^{0} \right) + \int_{298K}^{T} \left(C_{p,C0} + C_{p,H2} - C_{p,C} - C_{p,H20} \right) dT \right]$$
(47)

(t)

$$\Delta H_{T-(t)}^{0} = \left(\frac{x13_{d4}}{M_{H2}} - \frac{x14_{d5}}{M_{H20}}\right) \left[\Delta H_{H20}^{0} + \int_{298K}^{T} \left(C_{p,H20-g} - C_{p,02} - \frac{1}{2}C_{p,H2}\right) dT\right]$$
(48)

(u)

$$\Delta H_{T-(u)}^{0} = \frac{x l_{d5}}{M_{c}} \left[\left(\Delta H_{CO}^{0} - \Delta H_{C-S}^{0} \right) + \int_{298K}^{T} \left(C_{p,CO} - C_{p,C} - \frac{1}{2} C_{p,O2} \right) dT \right]$$
(49)

kd_{C-L} 0.025	<i>kdс</i> - <i>D</i> 35	<i>kdc</i> -1 60	<i>kdc</i> -2 55	<i>kdc-3</i> 0.035	<i>kdc-4</i> 0.0035
kd _{C-5}	kd _{C-6}	$kd_{gas-(q)}$	$kd_{gas-(r)}$	$kd_{gas-(s)}$	kdco-1
0.06	0.017	1.35	0.0006	0.065	0.95
kd _{Mn-1}	$kd_{H2-post}$	kd _{H2O}	kd _{CH4-post}	kd_{comb}	
1	0.1	1	5	0.028	

Table 2. Reaction rates used in the model. All rates are in kg s⁻¹.

Table 3. Fractions used in the model.

W02-air 0.23	^W N2-air 0.77	WN2-in-natgas 0.25	WCH4-in-natgas 0.75	WN2-in-oxygen 0.026	W02-in-oxygen 0.93
K _{leakair-02-CO(1)} 0.4	K _{leakair-02-CO(2)} 0.3	<i>K</i> _{02-C0} 0.15	<i>K</i> _{02-C02} 0.15	<i>K</i> _{02-post-C0} 0.01	
$K_{burn-(n1)}$ 0.55	<i>K</i> _{burn-(n2)} 0.3	<i>K</i> _{burn-(n3)} 0.15	$x_{(q)}$ 0.8	$\begin{array}{c} x_{(r)} \ 0.066 \end{array}$	$x_{(s)}$ 0.134

Table 4. Values of other parameters used in the model.

$\frac{K_{PR}}{0.3 \text{ kg s}^{-1}\text{Pa}^{-1}}$
<i>k</i> _u 6.44
_

695	kg	g mol ⁻¹ , $ ho_i$ in kg n	n^{-3} , $C_{p,i}$ in kJ mol	$^{-1}$ K ⁻¹ , ΔH_i^0 in kJ	mol ⁻¹ and λ_i in kJ	$(\text{mol}^{-1}).$
-	<i>M_C</i> 0.012	<i>M_{CO}</i> 0.028	<i>M</i> _{CO2} 0.044	$M_{N2} \ 0.028$	<i>M</i> ₀₂ 0.032	M_{H2} 0.002
	<i>M_{H2O}</i> 0.018	<i>М_{СН4}</i> 0.016	M_{Fe} 0.0559	M_{Si} 0.0281	<i>M</i> _{<i>Cr</i>} 0.052	M_{Mn} 0.0549
	<i>M</i> _P 0.031	<i>M_{FeO}</i> 0.0718	<i>M</i> _{<i>SiO2</i>} 0.0601	M_{MnO} 0.0709	<i>M</i> _{Cr203} 0.1520	<i>M</i> _{P205} 0.1419
	<i>M</i> _{AI203} 0.102	<i>M_{CaO}</i> 0.0561	<i>M_{MgO}</i> 0.0403	<i>М</i> с9н20 0.1283	M _{leakair} 0.0289	
	$C_{p,C} \ 0.0085$	$C_{p,CO} \\ 0.0291$	$C_{p,CO2} \\ 0.0381$	$C_{p,N2} \ 0.0291$	$C_{p,O2} \\ 0.0294$	$C_{p,H2} \ 0.029$
	$C_{p,H2O-g} \ 0.0342$	$C_{p,CH4}$ 0.035	$C_{p,Fe}$ 0.0251	$C_{p,Si}$ 0.0197	$C_{p,Cr}$ 0.0233	$C_{p,Mn}$ 0.0263
	$C_{p,P} \ 0.0212$	$C_{p,FeO}$ 0.048	$C_{p,SiO2}$ 0.0448	$C_{p,MnO}$ 0.0431	$C_{p,Cr2O3} \\ 0.1097$	$C_{p,P205}$ 0.2115
	$C_{p,C9H20} \ 0.2833$	$\begin{array}{c} C_{p,H2O\text{-}l} \\ 0.075 \end{array}$	$C_{p,sSc}$ 0.039	$C_{p,lSc}$ 0.047	$C_{p,sSl}$ 0.025	$C_{p,ISl}$ 0.047
	$C_{p,gas}$ 0.03	λ_{sSc} 15.4	λ _{sSI} 12.66	λ _C 117	<i>рсн4</i> 0.72	<i>ρco</i> 1.25
	<i>ρco</i> 2 1.98	<i>ρ</i> _{N2} 1.25	<i>ρο</i> ₂ 1.429	<i>р</i> _{<i>H</i>2} 0.0899	<i>р</i> _{<i>H20</i>} 0.59	
	ΔH^{0}_{C-S} -27	ΔH_{CO}^0 -117	ΔH_{CO2}^0 -396	ΔH^{0}_{H2O} -247	ΔH^{0}_{CH4} -91	ΔH^{0}_{C9H20} 2.256

Table 5. Used values of thermodynamical and physical substance constants (M_i in kg mol⁻¹, ρ_i in kg m⁻³, $C_{p,i}$ in kJ mol⁻¹ K⁻¹, ΔH_i^0 in kJ mol⁻¹ and λ_i in kJ mol⁻¹).

697 698	List of Captions		
699 700	Table caption	ons	
700 701	Table 1.	Enthalpy reactions.	
702	Table 2.	Reaction rates used in the model. All rates are in kg s ⁻¹ .	
703	Table 3.	Fractions used in the model.	
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705 706	Table 5.	Used values of thermodynamical and physical substance constants (M_i in kg mol ⁻¹ , ρ_i in kg m ⁻³ , $C_{p,i}$ in kJ mol ⁻¹ K ⁻¹ , ΔH_i^0 in kJ mol ⁻¹ and λ_i in kJ mol ⁻¹).	
707 708 709 710 711	Figure capti	ions ture and functioning of the EAE process model	
712	Fig. 2 Mass	ured (mass) and simulated (sim) mass fractions w of CO and COs in the off gas	
712	Fig. 2. Measured (meas) and simulated (sim) mass fractions w_i of CO and CO ₂ in the off-gas of a single heat.		
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723	Fig. 9. Averaged CO mass flows of the equilibrium reactions from Boudouard $(x9_{d7})$, the		

Fig. 9. Averaged CO mass flows of the equilibrium reactions from Boudouard $(x9_{d7})$, the heterogeneous water-gas reaction $(x9_{d9})$ and the homogeneous water-gas reaction $(x9_{d5})$.