

Article

Detailed Modeling of the Direct Reduction of Iron Ore in a Shaft Furnace

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Abstract: This paper addresses the modeling of the iron ore direct reduction process in the context of the reduction in CO₂ emissions from the steel industry. The shaft furnace is divided into three sections (reduction, transition, and cooling), and the model is two-dimensional (cylindrical geometry for the upper sections and conical geometry for the lower one) to correctly describe the lateral gas feed and the cooling gas outlet. This model relies on a detailed description of the main physical-chemical and thermal phenomena using a multi-scale approach. The moving bed is assumed to be comprised of pellets of grains and crystallites. Eight heterogeneous and two homogeneous chemical reactions are taken into account. The local mass, energy and momentum balances are numerically solved using the finite volume method. This model was successfully validated by simulating the shaft furnaces of two direct reduction plants of different capacities. The calculated results reveal the detailed interior behavior of the shaft furnace operation. Eight different zones can be distinguished according to their predominant thermal and reaction characteristics. An important finding is the presence of a central zone of lesser temperature and conversion.

Keywords: ironmaking; direct reduction; iron ore; DRI; shaft furnace; mathematical model; heterogeneous kinetics; heat and mass transfer.

1. Introduction

The direct reduction (DR) of iron ore, usually followed by electric arc steelmaking, is an alternative route to the standard blast furnace-basic oxygen furnace route for making steel. The annual DR iron production (86 Mt in 2017) remains small compared to the 1180 Mt of production of blast furnace pig iron [1]. However, an attractive feature of DR compared to blast furnace reduction is its much lower CO₂ emissions, which are 40 to 60% lower for the DR-electric arc furnace route compared to the blast furnace-basic oxygen furnace route [2]. Among the DR processes, the shaft furnaces represent over 82% of the world DR iron production, with the two main processes being MIDREX (see Fig. 1) (65%) and HYL-ENERGIRON (17%) [3].

In a DR shaft furnace, a charge of pelletized or lump iron ore is loaded into the top of the furnace and is allowed to descend by gravity through the reducing gas. The reducing gas, comprised of hydrogen and carbon monoxide (syngas) obtained by the catalytic reforming of natural gas, flows upwards through the ore bed. Reduction of the iron oxides occurs in the upper section of the furnace at a temperature up to 950°C. A transition section is found below the reduction section; this section is of sufficient length to separate the reduction section from the cooling section to allow an independent control of both sections. The solid product, called direct reduced iron (DRI) or reduced sponge iron, is cooled in the lower part of the furnace down to approximately 50°C prior to being discharged.

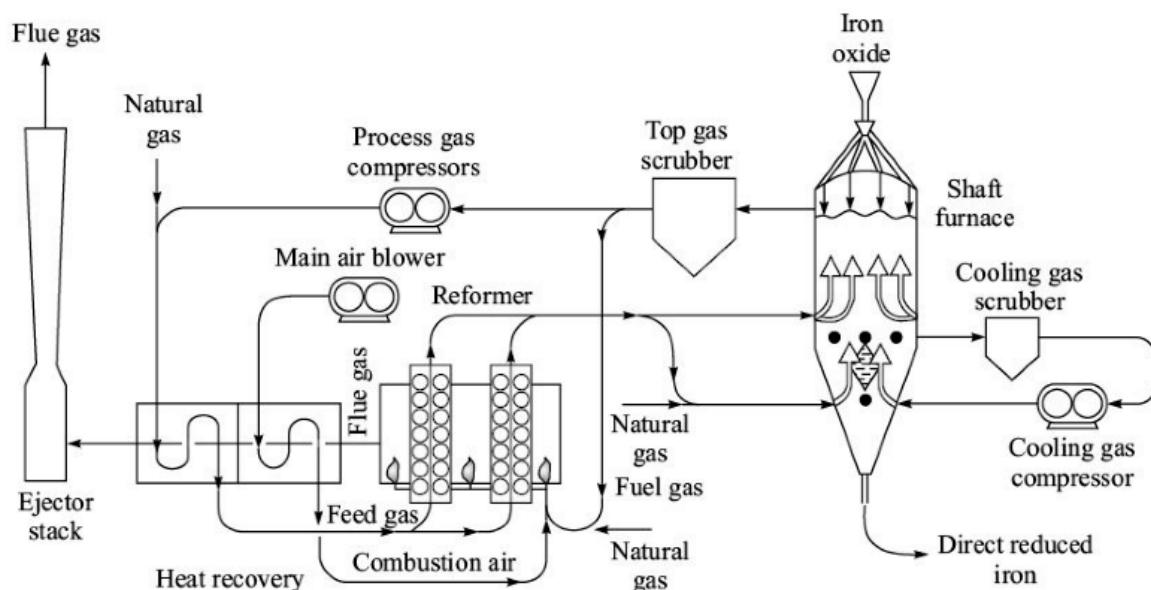


Figure 1. MIDREX process flowsheet [4]

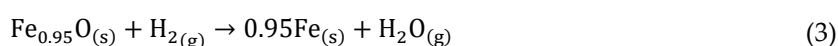
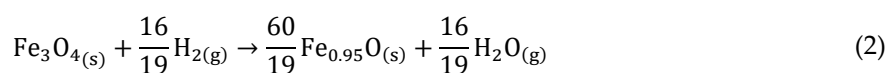
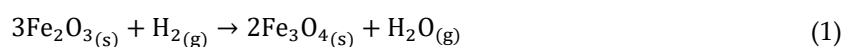
Modeling of a shaft furnace to simulate the reduction of iron ore by syngas is a powerful tool for defining the optimal operating conditions that lead to a maximization of the conversion or a minimization of the energy consumption, among other effects capable of reducing carbon dioxide emissions. Numerous iron ore shaft furnace models were thus proposed in the literature. The first studies addressed the reduction of a single pellet by H_2 , CO , or H_2 - CO mixtures [5-10]. The subsequent ones developed models that simulate the reduction zone of the shaft furnace in 1D [11-12]. With the aim to correctly describe the lateral gas feed, some studies introduced two-dimensional models [13-15]; however, these models did not consider the presence of methane, which is responsible for important reactions in the process, in the reducing gas. More recently, several authors introduced more reactions [16] and also accounted for the cooling zone [17-18] and some even developed plant models [19]; however, these works were limited to one-dimensional models.

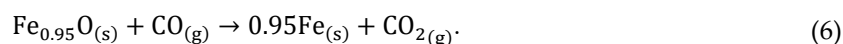
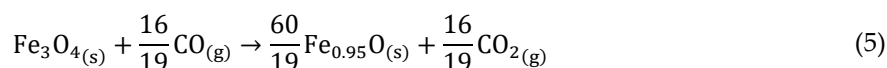
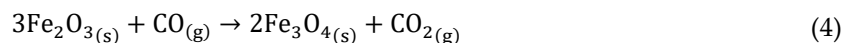
In this work, we further developed the model of Ranzani Da Costa and Wagner, built to simulate the reduction section of DR shaft operated with pure hydrogen [14, 15, 20], extending it to consider CO - H_2 - CH_4 reducing gas as well as accounting for the transition and cooling sections. The present model, named REDUCTOR, is 2-dimensional in the steady-state regime. The model includes a sophisticated pellet sub-model. Eight heterogeneous and two homogeneous chemical reactions are considered. These features represent a more advanced and detailed model compared to previous studies. Moreover, the results were validated against two sets of plant data.

2. Mathematical model

2.1. Principle

The reduction of the hematite ore to iron occurs via two intermediate oxides, namely, magnetite and wustite (considered as $Fe_{0.95}O$), and by two gaseous reactants, namely, H_2 and CO . The following six reduction reactions were therefore considered:





Methane reforming and water gas shift reactions also occur in the gas phase based on the composition of reduction gas and temperature through the following reactions:



We also considered two other side reactions that could occur in the reactor, especially where an iron layer has been formed:

- methane decomposition reaction



- carbon monoxide disproportionation (inverse Boudouard reaction)



The model itself is two-dimensional, axisymmetrical and steady-state. It is based on the numerical solution of the local mass, energy and momentum balances using the finite volume method. The geometry is cylindrical in the reduction and transition sections and conical in the cooling section. This corresponds to the geometry of the shaft furnaces and is necessary to describe correctly the lateral gas feed and outlet cooling gas (Fig. 2). The reactor modeled is a shaft furnace of the MIDREX type.

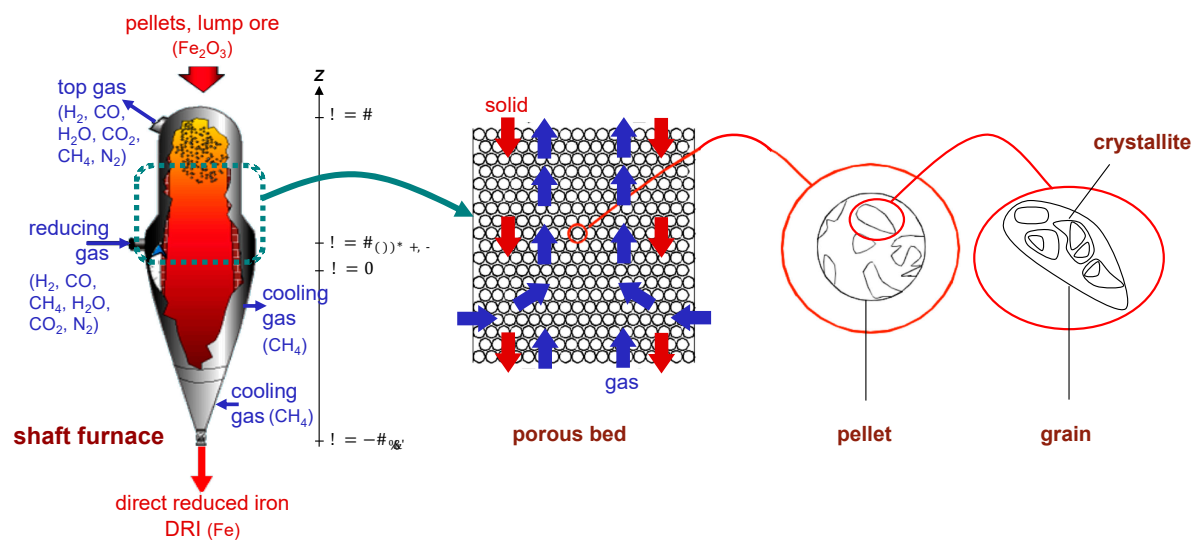


Figure 2. Schematic representation of the REDUCTOR model

The solid load is fed from the top of the reactor to form a moving bed of solid particles composed of spherical iron ore pellets that descend by gravity. The pellet diameter d_p is assumed to be unique and unchanging during the reduction reaction. The initial pellet composition is known. The gas phase is composed of six species (H_2 , CO , H_2O , CO_2 , N_2 and CH_4). The reducing gas is injected from the sidewall at a height of $z = H_{\text{Feed,gas}}$ and then moves upward against the solid flow before finally exiting the furnace at the top. The temperature and composition of this reducing gas are known. A secondary feed gas (cooling gas) introduced from the bottom of the furnace is also considered. This cooling gas exits the furnace through the wall in the upper part of the conical section. The

temperatures of the solid and the gas are different and vary according to the position (r, z) within the furnace. The solid temperature is assumed to be uniform in the interior of the pellets. This model is thus based on a faithful description of the physical-chemical and thermal phenomena, from the reactor scale to the crystallite scale (Fig. 2). In the pellet sub-model, the pellet is assumed to be initially comprised of dense grains; these grains later fragment into smaller crystallites at the wustite stage, in agreement with microscopic observations [20]. From the reactor to the crystallites, we thus have a 4-scale model.

2.2. Equations

2.2.1. Gas phase

The descending solid pellets through which the ascending gas flows can be considered as a porous medium consisting of quasi-stationary solid spheres (the gas velocity is much greater than that of the solid). The Ergun equation combined with the continuity equation thus gives (see Appendix A for the nomenclature)

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\frac{rc_t}{K} \frac{\partial p}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{c_t}{K} \frac{\partial p}{\partial z} \right) = S_{mol,tot} = 2r_7 + r_9 - r_{10} \quad (11)$$

where the terms are in units $mol\ m^{-3}\ s^{-1}$; K is the permeability coefficient, calculated as

$$K = \frac{150(1 - \varepsilon_b)^2}{\varepsilon_b^3 d_p^2} \mu_g + \frac{1.75(1 - \varepsilon)}{\varepsilon_b^3 d_p} \rho_g u_g \quad (12)$$

and the source term $S_{mol,tot}$ corresponds to the net gas production by the non-equimolar reactions. Equation (11) is used to calculate the pressure field, and the gas velocity vector is then calculated using Equation (13):

$$\mathbf{u}_g = -\frac{1}{K} \nabla P \quad (13)$$

The mass balance for a gaseous species i , considering axial and radial dispersion in addition to convection, is written:

$$\frac{1}{r} \frac{\partial (rc_t x_i u_{g,r})}{\partial r} + \frac{\partial (c_t x_i u_{g,z})}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left(rc_t D_r \frac{\partial x_i}{\partial r} \right) + \frac{\partial}{\partial z} \left(c_t D_z \frac{\partial x_i}{\partial z} \right) + S_i \quad (14)$$

with the source term S_i given in Table 1.

Table 1. Source terms for the gas species mass balances

Species i	S_i ($mol\ m^{-3}\ s^{-1}$)
H ₂	$S_{H_2} = -r_1 - \frac{16}{19}r_2 - r_3 + 3r_7 + r_8 + 2r_9$
CO	$S_{CO} = -r_4 - \frac{16}{19}r_5 - r_6 + r_7 - r_8 - 2r_{10}$
H ₂ O	$S_{H_2O} = r_1 + \frac{16}{19}r_2 + r_3 - r_7 - r_8$
CO ₂	$S_{CO_2} = r_4 + \frac{16}{19}r_5 + r_6 + r_8 + r_{10}$
CH ₄	$S_{CH_4} = -r_7 - r_9$

The heat balance for the gas phase, considering convection and conduction, as well as the heat exchanged with the solid and heat brought by the gases evolving from the solid, gives:

$$\rho_g c_{pg} \left(u_{gr} \frac{\partial T_g}{\partial r} + u_{gz} \frac{\partial T_g}{\partial z} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_g \frac{\partial T_g}{\partial r} \right) + \frac{\partial}{\partial z} \left(\lambda_g \frac{\partial T_g}{\partial z} \right) + a_b h (T_s - T_g) + \sum_i S_i \int_{T_g}^{T_s} c_{p_i} dT \quad (15)$$

2.2.2. Solid phase

Regarding the grain flow, in the upper cylindrical section, it is considered that the pellets descend vertically. In contrast, in the lower section of conical shape, a radial component of the solid velocity must be introduced. A bibliographical study of granular flows led us to use the model of Mullins [21, 22], where the radial velocity is calculated as being proportional to the radial gradient of the axial velocity:

$$u_{s,r} = -B \frac{\partial u_{s,z}}{\partial r} \quad (16)$$

where B is taken as proposed in [21]

$$B = 2d_p. \quad (17)$$

The mass balance for a gaseous species j gives:

$$-\frac{\partial(\rho_b u_{s,z} w_j)}{\partial z} + \frac{1}{r} \frac{\partial(r \rho_b u_{s,r} w_j)}{\partial r} = S_j \quad (18)$$

with the source term S_j given in Table 2:

Table 2. Source terms for the solid species mass balances

Species j	S_j ($kg\ m^{-3}\ s^{-1}$)
Fe_2O_3	$-3M_{Fe_2O_3}(r_1 + r_4)$
Fe_3O_4	$M_{Fe_3O_4}(2r_1 - r_2 + 2r_4 - r_5)$
$Fe_{0.95}O$	$M_{Fe_{0.95}O}\left(\frac{60}{19}r_2 - r_3 + \frac{60}{19}r_5 - r_6\right)$
Fe	$0.95M_{Fe}(r_3 + r_6)$
C	$M_c(r_9 + r_{10})$

The heat balance for the solid phase takes into account axial and radial convection and conduction, as well as heat exchange with the gas phase; the heat of the reactions is attributed to the solid phase, considering that all the reactions occur either inside the pellets (heterogeneous reactions) or at their surfaces (homogeneous reactions catalyzed by the solid); thus:

$$-\rho_b u_{s,z} c_{ps} \frac{\partial T_s}{\partial z} + \rho_b u_{s,r} c_{ps} \frac{\partial T_s}{\partial r} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \lambda_{eff,r} \frac{\partial T_s}{\partial r} \right) + \frac{\partial}{\partial z} \left(\lambda_{eff,z} \frac{\partial T_s}{\partial z} \right) + a_b h (T_g - T_s) + \sum_{n=1}^{10} (-r_n \Delta_r H_n) \quad (19)$$

2.3. Transport coefficients

The various transport coefficients $D_r, D_z, \lambda_{eff,r}$, and $\lambda_{eff,z}$ as well as other parameters like specific heats are calculated as functions of temperature and composition. Details regarding the relationships used are given in [23].

2.4. Reaction rates

2.4.1. Iron oxide reduction

Unlike most of the previous approaches published that are based on the shrinking core model (with one or three fronts separating the oxides in the pellet), we developed a specific pellet sub-model. The sub-model was built according to our experimental findings to simulate the reduction of a single pellet by H_2 -CO. The reaction rate is a function of the local reduction conditions (temperature and gas composition) inside the reactor. We used the law of additive reaction times [24], which considers the different resistances (chemical reaction, diffusion, external transfer) involved in series.

Therefore, the time required to attain a certain conversion is approximately the sum of the characteristic times τ_i [15, 24]. This sub-model was first developed for simulating the reduction by H_2 only (see [15] for details); we extended it for the reduction by CO. The characteristic times and the reaction rates are listed in Appendix B.

2.4.2. Methane reforming and water gas shift reactions

Methane reforming and water gas shift reactions are known to be catalyzed by iron or iron oxides [25, 26]; their rates are thus functions of the composition of the reduction gas, temperature, and mass of the catalyst. The methane reforming rate equation considering the forward and reverse reactions is given by Equation (20):

$$r_7 = k_7(1 - \varepsilon_b)(1 - \varepsilon_{interg}) \left(P_{CH_4} P_{H_2O} - \frac{P_{CO} P_{H_2}^3}{K_{eq,7}} \right) \tag{20}$$

The expression of the reaction rate constant k_7 is given in Table 3. Because the reforming of CH_4 was hardly observed on the iron oxide catalysts, as reported in the literature (Takahata et al., 2010), it was considered that such reforming only occurs with iron as a catalyst. We assumed that sufficient iron was formed at the outer of the pellet when the reduction degree exceeded 50%.

Similarly, the rate expression for the water gas shift reaction is given by Equation (21):

$$r_8 = k_8(1 - \varepsilon_b)(1 - \varepsilon_{interg}) \left(P_{CO} P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_{eq,8}} \right) \tag{21}$$

on Fe or $Fe_{0.95}O$ as catalysts and by Equation (22)

$$r_8 = k'_8 \rho_c (1 - \varepsilon_b)(1 - \varepsilon_{interg}) \left(P_{CO} P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_{eq,8}} \right) \tag{22}$$

on Fe_2O_3 or Fe_3O_4 as catalysts. Here, besides iron, the various iron oxides also catalyze the reaction. The corresponding expressions for k_8 and k'_8 are given in Table 3, according to [25, 26].

Table 3. Kinetics constants

Reactions	Reaction rate constants k_i	References
7	$k_7 = 392 \exp\left(\frac{6770}{RT}\right) \text{ (mol cm}^{-3}\text{s}^{-1}\text{)}$	[26]
8	Fe $k_8 = 93.3 \exp\left(-\frac{7320}{RT}\right) \text{ (mol cm}^{-3}\text{s}^{-1}\text{)}$	[26]
	$Fe_{0.95}O$ $k_8 = 1.83 \times 10^{-5} \exp\left(\frac{7.84}{RT}\right) \text{ (mol cm}^{-3}\text{s}^{-1}\text{)}$	[26]
	Fe_3O_4 $k'_8 = 2.683372 \times 10^5 \exp\left(-\frac{112000}{RT}\right) \text{ (mol kg}_{cat}^{-1}\text{s}^{-1}\text{)}$	[25]
	Fe_2O_3 $k'_8 = 4.56 \times 10^3 \exp\left(-\frac{88000}{RT}\right) \text{ (mol kg}_{cat}^{-1}\text{s}^{-1}\text{)}$	[25]
9	$k_9 = 16250 \exp\left(-\frac{55000}{RT}\right) \text{ (mol m}^{-3}\text{s}^{-1}\text{)}$	[17, 27]
10	$k_{10} = 1.8 \exp\left(-\frac{27200}{RT}\right) \text{ (mol m}^{-3}\text{s}^{-1}\text{)}$	[17, 27]
	$k'_{10} = 2.2 \exp\left(-\frac{8800}{RT}\right) \text{ (mol m}^{-3}\text{s}^{-1}\text{)}$	

2.4.3. Carbonization reactions

In the DR furnace, carbon can be formed either from methane decomposition (reaction 9) or from CO disproportionation (reaction 10). Both reactions are reversible, and the reverse reactions are functions of the carbon activity. The carbon activity was calculated from Chipman's relationship [28]:

$$\log a_c = \frac{2300}{T} - 0.92 + \left(\frac{3860}{T}\right)C + \log\left(\frac{C}{1-C}\right) \quad (23)$$

where C is the ratio of atom C to atom Fe. For sake of simplicity, we did not distinguish between C and Fe₃C in the solid, both being considered as C.

The rate equation of the methane decomposition reaction is given by Equation (24)

$$r_9 = \frac{k_9}{P_{H_2}^{0.5}} (1 - \varepsilon_b)(1 - \varepsilon_{interg}) \left(P_{CH_4} - \frac{P_{H_2}^2 a_c}{K_{eq,9}} \right) \quad (24)$$

The expression of the reaction rate constant k_9 included in equation (24) was determined from [17, 27] as listed in Table 3.

The rate equation of the carbon monoxide disproportionation reaction is given by Equation (25)

$$r_{10} = (k_{10} P_{H_2}^{0.5} + k'_{10})(1 - \varepsilon_b)(1 - \varepsilon_{interg}) \left(P_{CO}^2 - \frac{P_{CO_2} a_c}{K_{eq,10}} \right) \quad (25)$$

and the values of the reaction rate constants k_{10} and k'_{10} are also provided in Table 3 from the same references.

2.5. Boundary conditions

The balance equations need a set of associated boundary conditions to be solved. First, the temperature and composition of the solids and gases are assumed to be known (operating conditions) at their respective inlets (top for the solids, and bottom and side for the gas). In addition, because of axisymmetry and tight walls, one has:

$$\begin{aligned} &\text{- Symmetry axis: zero fluxes } \frac{\partial T_s}{\partial r} = \frac{\partial T_g}{\partial r} = \frac{\partial x_i}{\partial r} = 0 \\ &\text{- Side wall (except gas inlet): } \frac{\partial T_s}{\partial r} = \frac{\partial T_g}{\partial r} = \frac{\partial x_i}{\partial r} = 0 \end{aligned} \quad (26)$$

For the gas flow, a known pressure condition is also required at the exits. The top pressure was known but not the pressure of the outlet of cooling gas (point 4 in Fig. 3); the latter was estimated to obtain approximately 90% of inlet cooling gas exhausted from this outlet and approximately 10% flowing upwards.

Figure 3 shows the values of the known boundary conditions for the two simulations conducted, corresponding to two different plants. Plant A is a North American MIDREX plant currently in operation, the main operating data of which were provided to us. Plant B was the first MIDREX plant operated in the USA, for which published data are available [11]. The production capacity of plant A is 4.5 times greater than that of plant B.

2.6. Meshing and numerical solution

The system of partial derivative equations was discretized and solved according to the finite volume method [29]. Meshing of the cylindrical reduction and transition sections is orthogonal, with cells made finer next to the top (Fig. 4, left). For the conical section, a non-orthogonal grid was used (Fig. 4, right). To simply connect the two sections, the number of radial cells was kept the same. The numerical code was written in FORTRAN 1995 language.

3. Results and discussion

In this section, the results of plant A simulation are first presented and discussed, then a comparison between the calculated and measured data for both plants is given. The results for the

values of the different variables throughout the reactor are given in separate figures; however, all of these variables must be considered simultaneously for interpretation purpose.

3.1. Pressure field, velocity of gas and temperature field

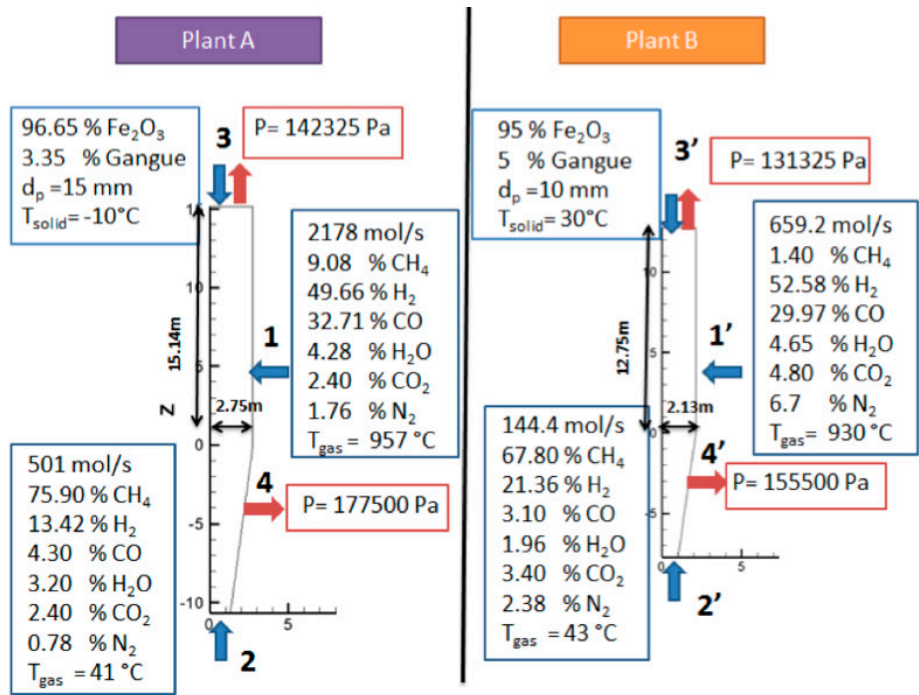


Figure 3. Operating conditions of plants A and B

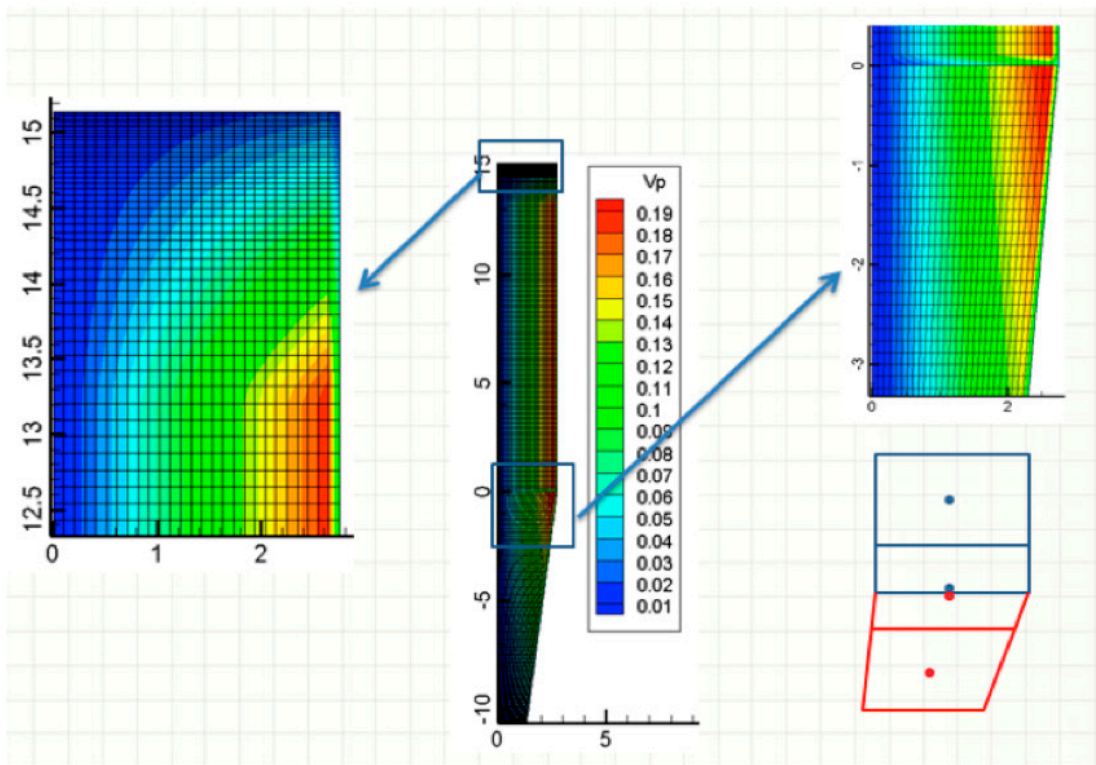


Figure 4. Meshing and volumes (m^3) of the cells

Figure 5 (a) shows the pressure and velocity fields inside the bed throughout the reactor. The color scale refers to the pressure, and the lines refer to the streamlines. The large arrows indicate the

locations of the various gas and solid inlets and outlets. These locations are the same (and not repeated everywhere) in the next figures. The pressure decreases almost linearly from bottom to top. The reducing gas injected at the sidewall ($z = 5.32$ m) enters radially and then flows essentially vertically upwards, except in the transition zone. The cooling gas first flows upwards, and then, most of it leaves the furnace radially at the cooling gas outlet, except for a fraction that rises in the reduction section.

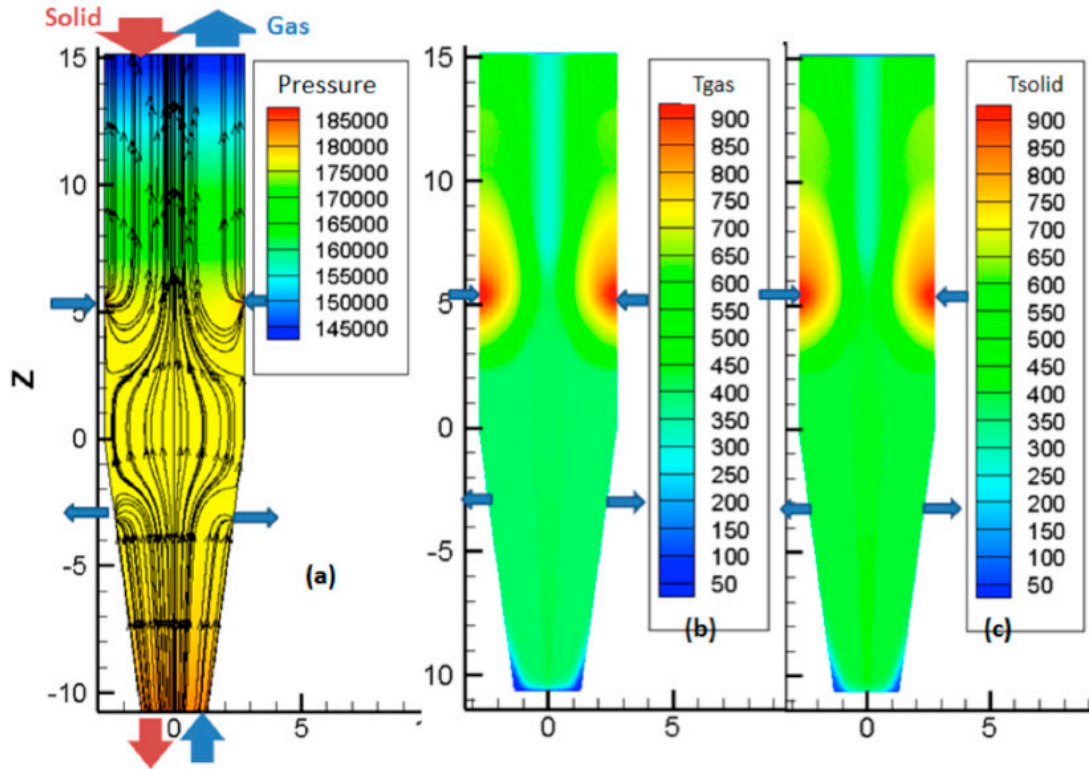


Figure 5. (a) Pressure field (Pa) and velocity streamlines of the gas flow inside the bed, (b) temperature distribution of the gas phase (°C), and (c) temperature distribution of the solid phase (°C).

Figures 5 (b) and (c) show the temperature distribution of the gas and solid phases in the reactor. First, it was found that the gas and solid temperatures are very close to each other. This similarity results from the high gas-to-solid heat transfer, as was already described by [15]. Downwards from the solid inlet, the solid temperature rapidly increases to reach the gas temperature. Second, the temperatures are not axially or radially uniform throughout the reactor. The hottest zone is near the reducing gas inlet, with gas introduced at 957 °C. Above this inlet, the temperature decreases because of methane reforming (as will be shown in Figure 7), an endothermic reaction. Third, the cooling gas not only cools the solid in the bottom section but also influences the temperature field in the reduction section, with the gas rising from the cooling zone to the central part of the reduction zone maintaining a lower temperature alongside the center of the shaft.

From these results, radial gradients of temperature are revealed that will influence, together with the gas composition profiles, the reduction of the solids and the metallization degree achieved.

3.2. Solid mass fractions

Figure 6 plots the evolution of the solid mass fractions throughout the reactor. Fig. 6 (a) shows that the hematite is fully converted to magnetite very rapidly in the upper part of the reactor. Subsequently, magnetite is reduced to wustite, as shown in Fig. 6 (b). Afterwards, wustite slowly begins to reduce to iron (Figs. 6 (c) and (d)). In the external two thirds of the reduction section, above the reducing gas inlet, a zone where the gas is rich in H_2 and CO and the temperature is high, the conversion to iron is completed in approximately 7 m. In the central part of the reactor, where the temperature is lower and the gas is poorer in H_2 and CO , the conversion is not completed and some

wustite remains in the cooling zone. Although the average metallization degree is approximately 94%, the metallization is not uniform, with most pellets being completely reduced, whereas others are not.

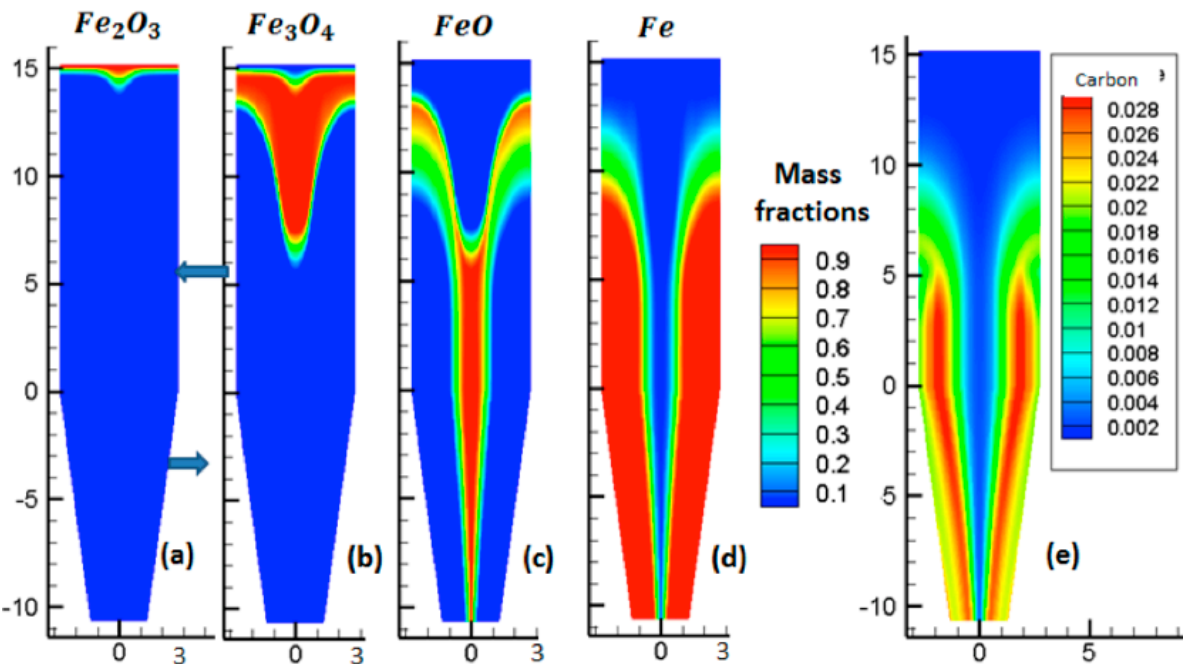


Figure 6. Mass fractions of the solid phases

Fig. 6 (e) shows the carbon mass fraction throughout the reactor. We observe that the carbon is in the same location as Fe, in accordance with the catalytic effect of iron on carbon formation.

3.3. Gas mole fractions

As showcased by Figure 7, the situation here is more complex, due to the numerous reactions occurring. The main features of these reactions are as follows. Near the reducing gas inlet, the reforming of methane occurs, which increases the H₂ and CO contents. Above the gas inlet, H₂ and CO contents decrease while H₂O and CO₂ are formed, as a result of the reduction reactions. In the central zone, with less reduction, lower amounts of H₂O and CO₂ are formed, and part of the cooling gas rich in CH₄ is present.

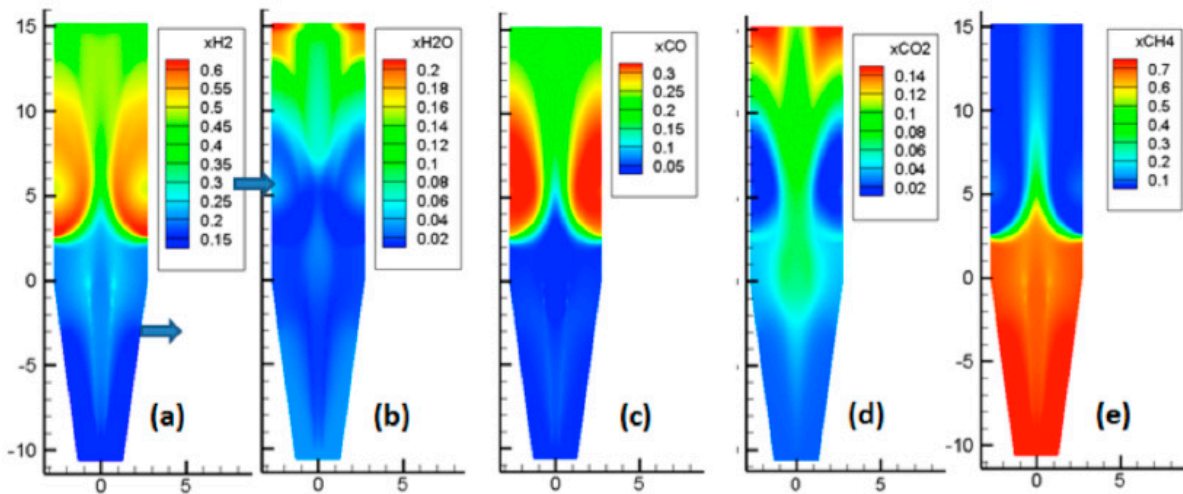


Figure 7. Mole fractions of the gas phase

3.4. Overall picture

Figure 8 is a summary diagram based on the above results. The shaft furnace was divided into eight zones, distinguished according to the main chemical and thermal processes occurring. On the left part of the diagram are also indicated the molar percentages of H₂ and CO involved in each reaction and the molar percentage of methane reformed by H₂O, CO₂ or decomposed to carbon and H₂. This diagram is an illustration of how modeling work can help to understand the detailed behavior of a reactor. Clearly, these results could not be obtained from other means.

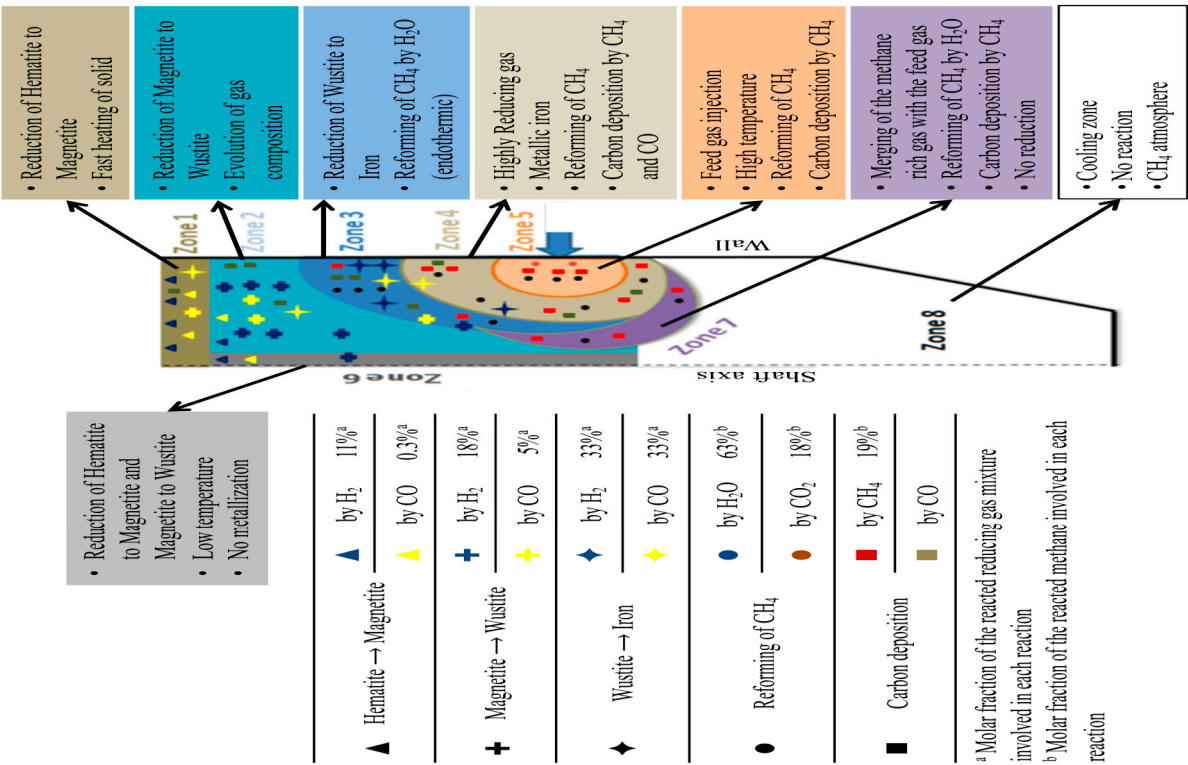


Figure 8. Diagram illustrating the different zones in the shaft furnace

3.5. Validation

Interior measurements of solid and gas temperatures and compositions are unfortunately not available for comparison with the calculations. However, from some published data regarding plant B and from plant data measurements from plant A, an overall validation of the model was possible.

Table 4 provides a comparison of the simulation results with the available plant data. It can be seen that the model reproduces the outlet temperatures and compositions quite satisfactorily. From this good agreement obtained with simulations of two plants of different capacities, the model can be considered as validated.

4. Conclusion

This article presented the modeling and simulation of an iron ore direct reduction shaft furnace. We developed a new mathematical model with the aim of introducing a more detailed description of the chemical processes compared to previous studies. The model is two-dimensional, describes three sections in the shaft, and accounts for eight heterogeneous and two homogeneous reactions. The model was validated against plant data from two MIDREX plants of quite different capacities. From the analysis of the calculated 2D maps of temperature and composition of the gas and solid phases, it was possible to gain new insights into the interior behavior of the shaft furnace to identify different

zones according to the chemical and thermal phenomena occurring. One significant result is the presence of a central zone of the shaft of lesser temperature and conversion. Such a model can also be helpful to optimize the whole reduction process, in particular, when the reducing gas characteristics are changed.

Table 4. Comparison of the Plant A and Plant B outlet data with the REDUCTOR model calculations

		Plant A		Plant B		
		Plant data	REDUCTOR Results	Plant data	REDUCTOR Results	Unit
Outlet solid	Composition (%)					
	Fe ₂ O ₃	0	0	0	0	wt %
	Fe ₃ O ₄	0	0	0	0	wt %
	FeO	7.47	7.1	n.a.	4.3	wt %
	Fe	85.72	85.9	n.a.	87.77	wt %
	C	2	2.2	2	0.91	wt %
	Gangue	4.71	4.8	6.3	7.02	wt %
	Production	119.2	119.8	26.4	27.33	t/h
Metallization	93.8	94	93	95.3	%	
Outlet gas	Flow rate	193	200	n.a.	54	kNm ³ /h
	Composition (%)					
	H ₂	40.28	40.41	37	37.72	vol %
	CO	19.58	19.89	18.9	20.87	vol %
	H ₂ O	19.03	19.52	21.2	20.61	vol %
	CO ₂	17.09	14.69	14.3	13.13	vol %
	CH ₄	2.95	3.91	8.6	7.67	vol %
	N ₂	1.02	1.55			vol %
Temperature	285	284	n.a.	285	°C	

Author Contributions: Conceptualization, Olivier Mirgaux and Fabrice Patisson; Investigation, Hamzeh Hamadeh, Olivier Mirgaux and Fabrice Patisson; Methodology, Hamzeh Hamadeh, Olivier Mirgaux and Fabrice Patisson; Project administration, Fabrice Patisson; Resources, Fabrice Patisson; Software, Hamzeh Hamadeh and Fabrice Patisson; Supervision, Olivier Mirgaux and Fabrice Patisson; Writing – original draft, Hamzeh Hamadeh; Writing – review & editing, Fabrice Patisson.

Funding: this research was supported by the French State through two programs ‘Investment in the future’: (i) one operated by French Environment and Energy Management Agency (ADEME), ‘Valorization of CO₂ in industry’, 2014-18, VALORCO, No 1382C0245; the authors thank Mrs. Nathalie Thybaud and Aïcha El Khamlichi, and the coordinator, Dr. Eric de Coninck; and (ii) one operated by the National Research Agency (ANR) and referenced by ANR-11-LABX-0008-01 (LabEx DAMAS).

Acknowledgments: The authors also express their thank to the staff of ArcelorMittal at Maizières-lès-Metz, France, and Contrecoeur, Canada, for encouragements, information and discussion, especially Drs. S. Bertucci, J. Borlée, T. Quatravaux, and J. Farley.

Conflicts of Interest: The authors declare no conflict of interest.

Appendix A – Notation

<i>Latin</i>	
<i>a_b</i>	specific area of the bed (m ² /m ³)
<i>a_c</i>	activity of carbon
<i>C_t</i>	total molar concentration of the gas (mol m ⁻³)
<i>C_{pg}</i>	molar specific heat of the gas (J mol ⁻¹ K ⁻¹)
<i>C_{ps}</i>	mass specific heat of the solid (J kg ⁻¹ K ⁻¹)

d_p	pellet diameter (m)
D	diffusion or dispersion (D_a, D_r) coefficient (m^2/s)
h	heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
H	height of the cylindrical section of the shaft (m)
H_{inf}	height of the conical section of the shaft (m)
K_{eq}	equilibrium constant
K	permeability coefficient ($kg\ m^{-3}\ s^{-1}$)
k	mass transfer coefficient, or reaction rate constant
M	molar weight ($kg\ mol^{-3}$)
p	gas pressure
P_i	partial pressure of component i (bar)
r	radius (m)
r	reaction rate ($mol\ m^{-3}\ s^{-1}$)
R	ideal gas constant ($J\ mol^{-1}\ K^{-1}$)
S	source term
T	temperature (K)
u	velocity ($m\ s^{-1}$)
w_j	mass fraction of solid j
X	degree of conversion
x_i	molar fraction of i in the gas
z	height (m)

Greek

$\Delta_r H$	heat of reaction ($J\ mol^{-1}$)
ε	porosity
τ	characteristic time (s)
λ	thermal conductivity ($W\ m^{-1}\ K^{-1}$)
μ_g	viscosity of the gas ($Pa\ s$)
ρ_g	mass density of the gas ($kg\ m^{-3}$)
ρ_b	mass density of the bed ($kg\ m_{bed}^{-3}$)
$\tilde{\rho}_j$	molar density of species j in the bed ($mol\ m_{bed}^{-3}$)

Subscripts

b	bed
c	catalyst
$cryst$	crystallite
$chem$	chemical
$diff$	diffusional
$interg$	intergranular
ini	initial
$intrac$	intra-crystallite
$interc$	inter-crystallite
∞	in the bulk gas
eff	effective (for the bed)
eq	at equilibrium
g	gas
$grain$	grain
p	pellet
r	radial
s	solid
z	axial

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Table B1. Kinetic sub-model of a single pellet. Expressions of the characteristic times and reaction rates. *i*: reaction number (see §2.1), *k*: H₂ or CO.

	Hematite → Magnetite	Magnetite → Wustite	Wustite → Iron
External transfer	$\tau_{ext,i} = \frac{\tilde{\rho}_{Fe_2O_3,ini} d_p}{18k_g c_t (x_{k,\infty} - x_{k,eq(i)})}$	$\tau_{ext,i} = \frac{8\tilde{\rho}_{Fe_3O_4,ini} d_p}{57k_g c_t (x_{k,\infty} - x_{k,eq(i)})}$	$\tau_{ext,i} = \frac{\tilde{\rho}_{Fe_{0.95}O} d_p}{6k_g c_t (x_{k,\infty} - x_{k,eq(i)})}$
Intergranular diffusion	$\tau_{diff,interg(i)} = \frac{\tilde{\rho}_{Fe_2O_3,ini} (d_p)^2}{72(D_{k,eff})_{interg,i} c_t (x_{k,\infty} - x_{k,eq(i)})}$	$\tau_{diff,interg(i)} = \frac{2\tilde{\rho}_{Fe_3O_4,ini} (d_p)^2}{57(D_{k,eff})_{interg,i} c_t (x_{k,\infty} - x_{k,eq(i)})}$	/
Intragranular diffusion	/	$\tau_{diff,intrag(i)} = \frac{2\tilde{\rho}_{Fe_3O_4,ini} (d_{grain,ini})^2}{57(D_{k,eff})_{intrag,i} c_t (x_{k,\infty} - x_{k,eq(i)})}$	/
Inter-crystallite diffusion	/	/	$\tau_{diff,interc(i)} = \frac{\tilde{\rho}_{Fe_{0.95}O} (d_p)^2}{24(D_{k,eff})_{interc,i} c_t (x_{k,\infty} - x_{k,eq(i)})}$
Intra-crystallite diffusion (solid phase)	/	/	$\tau_{diff,intrac(i)} = \frac{\tilde{\rho}_{Fe_{0.95}O} d_{cryst,ini}^2}{24D_{sol} (c_{ox,eq} - c_{ox,\infty})}$
Chemical reaction	$\tau_{chem,i} = \frac{\tilde{\rho}_{Fe_2O_3} d_{grain,ini}}{6k_i c_t (x_{k,\infty} - x_{k,eq(i)})}$	$\tau_{chem,i} = \frac{\tilde{\rho}_{Fe_3O_4} d_{grain,ini}}{2k_i c_t (x_{k,\infty} - x_{k,eq(i)})}$	$\tau_{chem,i} = \frac{\tilde{\rho}_{Fe_{0.95}O} d_{cryst,ini}}{2k_i c_t (x_{k,\infty} - x_{k,eq(i)})}$

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Reaction <i>i</i>	Reaction rate $mol\ m^{-3}\ s^{-1}$
<i>i</i> =1 and 4	$r_i = \frac{1}{3} \tilde{\rho}_{Fe_2O_3,ini} \left\{ \tau_{ext,i} + 2\tau_{diff,interg(i)} \left[(1 - X_i)^{\frac{1}{3}} - 1 \right] + \frac{\tau_{chem,i}}{3} (1 - X_i)^{\frac{2}{3}} \right\}^{-1}$
<i>i</i> =2 and 5	$r_i = \frac{1}{3} \tilde{\rho}_{Fe_2O_3,ini} \left\{ \tau_{ext,i} + 2(\tau_{diff,interg(i)} + \tau_{diff,intrag(i)}) \left[(1 - X_i)^{\frac{1}{3}} - 1 \right] + \frac{\tau_{chem,i}}{3} (1 - X_i)^{\frac{2}{3}} \right\}^{-1}$
<i>i</i> =3 and 6	$r_i = \frac{1}{3} \tilde{\rho}_{Fe_2O_3,ini} \left\{ \tau_{ext,i} + 2(\tau_{diff,interc(i)} + \tau_{diff,intrac(i)}) \left[(1 - X_i)^{\frac{1}{3}} - 1 \right] + \frac{\tau_{chem,i}}{3} (1 - X_i)^{\frac{2}{3}} \right\}^{-1}$

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