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**Abstract**: Given the urgent pursuit of carbon neutrality and stringent climate policies, the  $H_2$  shaft furnace ( $H_2$ -SF) is starting to gain widespread attention in the steel industry. In this study, the performance of the  $H_2$ -SF under operation with a dual-row injection top gas recycling system was investigated by a one-dimensional mathematical model. The potential of microwave heating as a means to supply thermal energy in regions of energy deficit was also assessed briefly. The results showed that for scenarios without microwave heating, increasing the upper-row injection rate can improve the furnace performance, and increasing the distance of the upper-row injection level from the furnace top also has a positive effect. A high microwave heating efficiency is expected in regions above the upper-row injection level. For scenarios with microwave heating, a higher microwave power leads to a better furnace performance. Thus, a higher furnace productivity can be achieved by increasing either the upper-row injection rate or the microwave power. However, the latter seems more promising as it decreases the total energy demand due to a better utilization of thermal energy. Based on the comparison of two representative examples, the decrease in the total energy demand is about 0.2 GJ/t-Fe.

**Keywords:** H<sub>2</sub> shaft furnace; energy demand; dual-row injection; microwave heating; sustainable steelmaking

## 1. Introduction

Steel is undisputedly a central material component for modern societies, and its global demand is forecast to reach 2500 million tons in 2050 [1], mainly driven by population growth together with infrastructure construction/improvement in developing countries. At present, the dominant steelmaking route involves the coal-based blast furnace, where coke is used as a fundamental raw material for providing the reduction potential, permeability for the gas flow in the upper part of the furnace and liquid flow in the lower part, as well as carbon for the hot metal. Consequently, steelmaking today has a specific emission of approximately 1.9 t-CO<sub>2</sub>/t-steel and accounts for 7% of the global anthropogenic CO<sub>2</sub> emissions [2]. Given the urgent pursuit of carbon neutrality and stringent climate policies, the steel industry must significantly reduce its carbon footprint via adopting novel sustainable steelmaking technologies. Under these circumstances, hydrogen (H<sub>2</sub>) has gained rapidly rising popularity [3–5] as a reductant of iron ore with no other emissions than water vapor (H<sub>2</sub>O). Several pilot projects of H<sub>2</sub>-based steelmaking are currently underway, such as HYBRIT in Sweden [6] and  $\mu$ DRAL in Germany [7].

In essence, the  $H_2$ -based steelmaking chain runs on electricity and mainly consists of three sub-processes:  $H_2$  reduction (for converting iron oxide pellets to direct reduced iron, DRI), electric heating (for melting DRI and steelmaking) and water electrolysis (for generating  $H_2$ ). These are in practice realized using a direct reduction shaft furnace



**Citation:** Yu, S.; Shao, L.; Zou, Z.; Saxén, H. A Numerical Study on the Performance of the H<sub>2</sub> Shaft Furnace with Dual-Row Top Gas Recycling. *Processes* **2021**, *9*, 2134. https:// doi.org/10.3390/pr9122134

Academic Editor: Haiping Zhu

Received: 24 October 2021 Accepted: 23 November 2021 Published: 26 November 2021

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**Copyright:** © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). operated with pure H<sub>2</sub> (H<sub>2</sub>-SF), an electric arc furnace (EAF) as well as a (large-scale) electrolyzer, respectively. By utilizing clean (e.g., wind, solar or even nuclear) energy-based electricity, the specific emission of this new steelmaking route may be reduced to  $0.05 \text{ t-CO}_2/\text{t-steel}$  [8], with emissions mainly from the injection of carbon for refinement of liquid steel and the inevitable consumption of graphite electrodes in the EAF. In light of its substantial emissions-reduction potential, the H<sub>2</sub>-based steelmaking route is starting to gain worldwide acceptance, simultaneously leading to pioneering studies mostly focused on key issues including (1) assessment of the process economics and (2) understanding and then improvement of the H<sub>2</sub>-SF performance.

The first issue is of unequivocal importance since the production cost determines whether the process is commercially competitive, even though an extensive access to clean energy is foreseeable in the future. Vogl et al. [8] were among the first who assessed the H<sub>2</sub>-based steelmaking route in terms of energy demand and production cost. It was reported that the entire process needs 3.48 MWh of electricity to produce one ton of liquid steel, and the total production cost is highly sensitive to the price of electricity. The H<sub>2</sub>based route becomes economically viable only if electricity costs less than 20 EUR/MWh. When the  $CO_2$  emission tax is higher than 62 EUR/t- $CO_2$ , however, the new route tends to be competitive with the conventional blast furnace (basic oxygen furnace) route at an electricity price of less than 40 EUR/MWh. It is interesting to note that the present  $CO_2$ emission tax in the European Union is approaching the mentioned threshold value, but the electricity price is far higher than 40 EUR/MWh. As for the second issue regarding  $H_2$ -SF performance, due attention is required since the use of pure  $H_2$  introduces new challenges owing to the endothermic nature of H<sub>2</sub> reduction of iron oxides. In principle, utilization of chemical energy of the gas in the  $H_2$ -SF is poor since an excessively large amount of  $H_2$  is needed as a carrier of thermal energy ("sensible heat") in order to meet the considerable heat demand of the endothermic reactions and heating of the burden in the furnace. Ranzani da Costa et al. [9] built a mathematical model based on a description of the local mass, energy and momentum balances for the gas and solid species in a H<sub>2</sub>-SF. The simulation results showed that complete conversion of the (100% hematite) pellets to metallic iron (i.e., a DRI metallization degree of 1.0) is obtained in the furnace if a preheated H<sub>2</sub> (98%) + H<sub>2</sub>O (2%) gas stream of 1073 K is injected at a specific flow rate of 1609 Nm<sup>3</sup>/t-pellet. It can be further calculated that the top gas utilization degree (i.e., mole fraction of  $H_2O$  in the gas mixture consisting of  $H_2O$  and  $H_2$ ) is roughly 0.27 under the operating conditions considered. The present authors [10] also developed a H<sub>2</sub>-SF model and predicted that the top gas utilization degree is generally lower than 0.25 for scenarios where pure H<sub>2</sub> is injected into the furnace and the target DRI metallization degree is (close to) 1.0. In a recent publication [11], the study was extended to a new top gas recycling (TGR) concept featuring dual-row injection as an alternative way of relaxing the strong constraints imposed by the need to supply a large portion of thermal energy to the process. This preliminary assessment confirmed that the dual-row injection TGR system could improve the furnace performance, especially in terms of gas utilization degree and total energy demand. Recently, the state-of-the-art technology of microwave heating that has attracted widespread attention in the field of pyro-metallurgy [12,13] has appeared as an option of supplying thermal energy to the H<sub>2</sub>-SF. However, there is so far very little information on the use of microwave heating in shaft furnaces.

With the above motivations, the current work aims to clarify whether a better  $H_2$ -SF performance can be achieved using a combination of the dual-row injection TGR system and microwave heating technology. For this, a thorough numerical study was first carried out to determine a proper level of the upper-row injection, above which a microwave heater is installed. After studying this, the potential of microwave heating was assessed preliminarily by investigating the effects of microwave power. The findings of this work may serve as guidelines for future design of the  $H_2$ -SF as well as for carrying out optimization of existing syngas-based units.

# 2. Modeling

## 2.1. H<sub>2</sub>-SF Process

Figure 1 schematically depicts the  $H_2$ -SF with a microwave heater and configuration of the dual-row injection TGR system. As can be seen, the off-gas from the furnace top is passed through a dry deduster (i.e., A in Figure 1) followed by a (counter-flow) heat exchanger (B), into which a stream of (room-temperature) fresh  $H_2$  generated by an electrolyzer (H) is simultaneously introduced. Thus, the off-gas is dedusted and cooled, while the fresh  $H_2$  is preheated. By using a distributor (C), the former gas stream is split into two streams, one of which is compressed in a compressor (F2), heated in a heater (G2) and finally injected into the furnace at a higher (i.e., upper-row injection) level, while the other stream is introduced into a condenser (D) for removing  $H_2O$  to recover the remaining  $H_2$ . The recovered  $H_2$  is then blown into a mixer (E), together with the preheated fresh  $H_2$  from the heat exchanger (B). After mixing, the gas is compressed (F1), heated (G1) and finally injected into the furnace at a lower-row injection level. In addition, a microwave heater (*J*) with a height of *U* is installed above the upper-row injection, as also depicted in Figure 1.



**Figure 1.** Schematic of the H<sub>2</sub>-SF with a microwave heater and configuration of the dual-row injection TGR system.

## 2.2. H<sub>2</sub>-SF Model

The H<sub>2</sub>-SF model is similar to the one employed in the previous work where the potential of the dual-row injection TGR system was assessed, except for some extensions made to incorporate the effects of microwave heating. For the sake of simplification, the energy that the solid phase can effectively absorb under microwave heating is considered to decrease with the mass fraction of metallic iron in the solid. This is motivated by the fact that metals reflect microwaves and cannot be heated efficiently. In the following, only the key treatment and governing equations of the model are outlined: the reader is referred to Shao et al. [10] for detailed information about it.

The mathematical model was built based on a description of the complex gas–solid countercurrent reactive flow in the reduction zone of the furnace (cf. Figure 1). The gas

phase consists of five species: CO, H<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O and N<sub>2</sub>, and the solid phase contains Fe<sub>2</sub>O<sub>3</sub>, Fe<sub>3</sub>O<sub>4</sub>, wustite (Fe<sub>x</sub>O, *x* = 0.95), Fe as well as inert gangue components (being mainly CaO, SiO<sub>2</sub>, MgO and Al<sub>2</sub>O<sub>3</sub>). At a temperature above 849 K, the solid iron oxides are reduced by CO and H<sub>2</sub> following three consecutive steps: Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Fe<sub>3</sub>O<sub>4</sub>, Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  Fe<sub>x</sub>O and Fe<sub>x</sub>O  $\rightarrow$  Fe. When the temperature is below 849 K, the reduction occurs in two consecutive steps: Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Fe<sub>3</sub>O<sub>4</sub> and Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  Fe, since Fe<sub>x</sub>O is unstable at low temperatures. It is obvious that the model can be used to simulate the operation of H<sub>2</sub>-SF by simply setting the contents of CO, CO<sub>2</sub> and N<sub>2</sub> in the feed gas equal to zero.

Algebraic manipulation of the local mass, energy and momentum balances of the gas and solid phases gives rise to a set of coupled nonlinear ordinary differential equations (ODEs) for the gas temperature ( $T_g$ ), mole fraction of gaseous species ( $Y_i$ , i = 1, ..., 4representing H<sub>2</sub>, CO, H<sub>2</sub>O and CO<sub>2</sub>), solid temperature ( $T_s$ ), reduction degree of the reduction steps ( $X_j$ , j = 1, ..., 4 denoting reduction steps Fe<sub>2</sub>O<sub>3</sub>  $\rightarrow$  Fe<sub>3</sub>O<sub>4</sub>, Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  Fe<sub>x</sub>O, Fe<sub>x</sub>O  $\rightarrow$  Fe and Fe<sub>3</sub>O<sub>4</sub>  $\rightarrow$  Fe) as well as gas pressure ( $P_g$ ).

The gas temperature is given by:

$$\frac{\mathrm{d}T_{\mathrm{g}}}{\mathrm{d}z} = \frac{6(1-\varepsilon)}{d_{\mathrm{p}}} \frac{S}{\rho_{\mathrm{g}}G} \frac{h_{\mathrm{P}}}{C_{\mathrm{g}}} (T_{\mathrm{g}} - T_{\mathrm{s}}) + \frac{\pi D}{\rho_{\mathrm{g}}G} \frac{h_{\mathrm{w}}}{C_{\mathrm{g}}} (T_{\mathrm{g}} - T_{\mathrm{a}}) \tag{1}$$

where *z* is the vertical downward direction (cf. Figure 1). The variables  $\varepsilon$ ,  $d_p$ , *S*,  $\rho_g$ , *G*,  $C_g$ , *D*,  $h_p$ ,  $h_w$  and  $T_a$  are the bed porosity, pellet diameter, cross-sectional area of the reduction zone, density of gas, volumetric flow rate of gas, specific heat capacity at constant pressure, inner diameter of the reduction zone, gas–solid heat transfer coefficient, overall heat transfer coefficient over the furnace wall as well as ambient temperature, respectively.

The mole fractions of the gas species are obtained from:

$$\frac{dY_i}{dz} = \frac{6(1-\varepsilon)}{\pi d_p^3} \frac{S}{n_g} \sum_{i=1}^4 \alpha V_{i,i}, \begin{cases} \alpha = 1, \text{ if } i \le 2\\ \alpha = -1, \text{ if } i > 2 \end{cases}$$
(2)

where  $n_g$  and V are the molar flow rate of gas and the reduction rate of a single pellet.

In the above equation, *V* is computed using the widely accepted multi-step unreacted shrinking core model (see Hara et al. [14] for a thorough description).

The burden temperature is given by:

$$\frac{dT_s}{dz} = \frac{6(1-\varepsilon)}{d_p} \frac{S}{W} \frac{h_p}{C_s} (T_g - T_s) - \frac{6(1-\varepsilon)}{\pi d_p^3} \frac{S}{W} \frac{1}{C_s} \sum_{i=1}^2 \sum_{j=1}^4 V_{i,j} \Delta H_{i,j} - \frac{S}{W} \frac{\varepsilon}{C_s} V_{wg} \Delta H_{wg} + \frac{\lambda(1-\omega_{Fe})}{U} \frac{S}{W} \frac{1}{C_s} E_{mw}$$
(3)

where W,  $C_s$ ,  $\Delta H$ ,  $V_{wg}$  and  $\Delta H_{wg}$  are the mass flow rate of solid, specific heat capacity of solid, reaction enthalpy of each reduction step, reaction rate and enthalpy of the water gas shift reaction, respectively. The rightmost term in the equation represents the energy that the solid phase absorbs by microwave heating. The variables  $\lambda$ ,  $\omega_{Fe}$  and  $E_{mw}$  are the efficiency factor of the heater, mass fraction of metallic iron in the solid phase and power of the microwave heater, respectively. It should be noted that  $E_{mw}$  is nonzero only in the region covered by the microwave heater.

The reduction degrees of the iron oxides are given by:

$$\frac{\mathrm{d}X_j}{\mathrm{d}z} = \frac{6(1-\varepsilon)}{\pi d_{\mathrm{p}}^3} \frac{S}{W\beta_j \kappa} \sum_{i=1}^2 V_{i,j} \tag{4}$$

where  $\beta$  and  $\kappa$  are the initial oxygen mole fraction of each iron oxide and the total reducible oxygen content of the initial pellet.

Finally, the gas pressure is given by:

$$\frac{dP_g}{dz} = 150 \frac{(1-\varepsilon)^2}{\varepsilon^3} \frac{\mu_g u_g}{d_p^2} + 1.75 \frac{(1-\varepsilon)}{\varepsilon^3} \frac{\rho_g u_g^2}{d_p}$$
(5)

where  $\mu_g$  and  $u_g$  are the dynamic viscosity and superficial velocity of the gas.

For the two-point boundary conditions that result from the nature of the countercurrent flows, the solution of the ODEs can be found by a shooting method. For detailed information about the numerical method, the reader is referred to Shao et al. [10]. The total energy demand of the entire process is the sum of the energy demand of electrolysis, compression and heating. In the computation of the last term, the recycled heat for preheating the fresh  $H_2$  in the counter-flow heat exchanger is subtracted. The reader is referred to Karwa [15] for the effectiveness NTU (number of transfer units) method, which is used to estimate the recycled heat in the counter-flow heat exchanger (cf. B in Figure 1).

## 2.3. Model Parameters

The main parameters used in the model are provided in this section. Table 1 presents the correlations used for the chemical reaction rate constants and effective diffusion coefficients concerning  $H_2$  reduction of the pellets considered in the model [16]. Table 2 presents the geometry parameters and the boundary conditions of the model, while Table 3 reports parameters needed for the evaluation of the energy demand of the system.

**Table 1.** Correlations [16] of chemical reaction rate constant (k) and effective diffusion coefficient ( $D_{\text{eff}}$ ) concerning H<sub>2</sub> reduction of the pellets considered in the model.

<b>Reduction Step</b>	Correlation for <i>k</i> , cm/s	Correlation for D <sub>eff</sub> , cm <sup>2</sup> /s
$\begin{array}{c} Fe_2O_3 \rightarrow Fe_3O_4 \\ or \\ Fe_3O_4 \rightarrow Fe \end{array}$	$\exp\left(4.49 - \frac{33.4}{RT_{\rm s}}\right)$	$\exp\left(3.43 - \frac{4.2 \times 10^3}{T_{\rm s}}\right)$
$Fe_3O_4 \rightarrow Fe_xO$	$\exp\left(6.70 - \frac{58.2}{RT_s}\right)$	$\exp\!\left(5.64 - rac{6.8  imes 10^3}{T_{ m s}} ight)$
$Fe_xO \to Fe$	$\exp\left(6.97 - rac{57.1}{RT_{ m s}} ight)$	$\exp\!\left(4.77-rac{5.9 imes10^3}{T_{ m s}} ight)$

Table 2. Key specifications and model parameters of the H<sub>2</sub>-SF in this work.

Parameter (Symbol)	Value	Parameter (Symbol)	Value
Length of reduction zone ( <i>L</i> )	5.0 m	Pellet composition - (T.Fe, FeO, CaO, SiO <sub>2</sub> , MgO, Al <sub>2</sub> O <sub>3</sub> , Rest)	64.60, 0.26, 0.26, 3.71, 0.14, 2.18, 1.45 wt.%
Diameter of reduction zone (D)	3.5 m		
Pellet diameter $(d_p)$ and bed porosity $(\varepsilon)$	14.0 mm, 0.4	Top gas pressure $(P_{g,0})$	1.5 bar
Solid feed rate $(W_0)$	100 t/h	Gas feed temperature $(T_{g,L} \text{ and } T_{g,H})$	1173 K
Solid feed temperature $(T_{s,0})$	298 K	Lower-row injection rate $(G_L)$	1200 Nm <sup>3</sup> /t-pellet
Initial reduction degree of solid $(X_{total,0})$	0	Lower-row gas composition (H <sub>2</sub> , H <sub>2</sub> O)	100.0 vol.%

Table 3. Parameters for assessment of the energy demand.

Parameter	Value
Energy demand of electrolyzer	$4.9 \text{ kWh/Nm}^3$ -H <sub>2</sub>
Efficiency factor of compressor	0.7
Efficiency factor of gas heater	0.7
Efficiency factor of microwave heater	0.7
NTU of heat exchanger	5.0
Outlet temperature of condenser	343 K

## 2.4. Model Validation

In earlier work by the authors [10], the model was validated by comparing its predictions with measured data from a small-scale syngas-based shaft furnace [17,18], showing a reasonable overall agreement. To further assess the accuracy of the model, industrial production data of a MIDREX shaft furnace (Gilmore plant) reported by Parisi and Laborde [19], and later by Shams and Moazeni [20], were used. The reported length and inner diameter of the reduction zone of the industrial furnace are 9.75 and 4.26 m respectively, and the (volumetric) flow rate of the feed gas is  $53,863 \text{ Nm}^3/h$ . The temperature and species mole fractions of the feed gas are 1203 K and 52.58% H<sub>2</sub>, 29.97% CO, 4.65% H<sub>2</sub>O, 4.8% CO<sub>2</sub> and 8.1% CH<sub>4</sub> + N<sub>2</sub>, respectively. For the sake of simplicity, however, the CH<sub>4</sub> was neglected here and the mole fraction of  $N_2$  was set equal to 8.1% in the simulation presented in this section. In addition, the DRI production rate is 26.4 t/h, with an average metallization degree of 0.93. According to Shams and Moazeni [20], the required solid feed rate is about 37.3 t/h, assuming that the pellets contain 95% Fe<sub>2</sub>O<sub>3</sub> and 5% gangue. Thus, the specific gas feed rate can be estimated to be 1444 Nm<sup>3</sup>/t-pellet. For other information about the industrial shaft furnace, the reader is referred to Parisi and Laborde [19] and Shams and Moazeni [20].

Figure 2 compares the mole fractions of gaseous species in the top gas as well as the DRI metallization degree reported by the authors with the corresponding values predicted by the model of the present work. As seen in the figure, the model can accurately predict the production data.



**Figure 2.** Comparisons between model prediction and industrial production data related to gaseous species in the top gas [19].

#### 3. Results and Discussion

#### 3.1. Effect of Upper-Row Injection Level

Numerical simulations were first conducted to elucidate the H<sub>2</sub>-SF performance for different distances (*H*) of the upper-row injection level from the furnace top (i.e., from the level of z = 0 m, cf. Figure 1) and different injection rates (*G<sub>H</sub>*) with the intent to determine a proper injection level above which the microwave heater should be installed.

As revealed in Figures 3 and 4, an increase in  $G_H$  yields an increase in both top gas utilization degree and DRI metallization degree. The underlying reason is that a higher  $G_H$  increases the supply of sensible heat to the furnace without deteriorating the in-furnace thermochemical state, since the reduction potential of the gas injected at the upper row is sufficient.



**Figure 3.** Effect of upper-row injection distance (*H*) on top gas utilization degree at different injection rates ( $G_H$ ).



**Figure 4.** Effect of upper-row injection distance (*H*) on DRI metallization degree at different injection rates ( $G_H$ ).

More interestingly, Figures 3 and 4 show that increasing the distance of the upper injection level from the top, H, can also improve the two key performance indices, although the extent is lesser. This is chiefly attributed to the fact that a longer zone facilitates a more efficient heat exchange between the ascending high-temperature injection gas and the descending solids. However, for a given  $G_H$ , the two indices are observed to grow only marginally for H > 3.5 m. Thus, the condition  $H \approx 3.5$  m corresponds to a close-to-limit gas–solid exchange. Since a deeper injection point also leads to a higher pressure drop of the gas, the total energy demand increases because more energy is required to compress the gas. Therefore, H = 3.5 m is taken as a proper position of the upper-row injection under the operating conditions considered in this work.

In order to substantiate the above arguments, the distributions of burden temperature (Figure 5a) and mass fraction of metallic iron (Fe) in the burden (Figure 5b) under the conditions of Cases 1–2 (cf. Figure 4) are compared in Figure 5a, showing that the burden temperature is increased in the lower parts of the shaft as upper-row injection is shifted downward from H = 1.5 m (Case 1) to H = 3.5 m (Case 2). This is obviously beneficial for the endothermic reduction reaction and thus results in a higher DRI metallization

degree, i.e., an increased mass fraction of Fe in the solid for Case 2, as depicted in Figure 5b. Moreover, the results indicate that a high microwave heating efficiency is expected in the region above H = 3.5 m, where only a little Fe, reflecting the microwaves, is present in the burden. This justifies the arrangement depicted in Figure 1, where the microwave heater is positioned above the upper-row injection level.



**Figure 5.** Distributions of solid temperature (**a**) and mass fraction of metallic iron (Fe) in the burden (**b**) under the conditions of two representative cases.

It is worth noticing that the DRI metallization degree under the conditions of Case 2 is still only about 0.82 (cf. Figure 4), which is much lower than the target value (i.e., 0.96) suggested by Duarte [21] for the H<sub>2</sub>-based steelmaking chain in terms of overall CO<sub>2</sub> emissions. However, the metallization degree can be raised to almost unity by increasing  $G_H$  to 750 Nm<sup>3</sup>/t-pellet, as seen in Case 3 of Figure 4.

## 3.2. Potential of Microwave Heating

Simulations were conducted for scenarios where the H<sub>2</sub>-SF is equipped with a combination of the dual-row injection TGR system and the microwave heater to assess the potential of microwave heating to improve the performance of the unit. Being a preliminary study, only the effects of microwave power ( $E_{mw}$ ) are investigated here, while sensitivity analyses of more factors will be left for future studies. The microwave heating height was chosen as U = 2.0 m and the remaining modeling parameters are identical to the ones used in Case 2.

From a theoretical point of view, heating the burden by using microwaves facilitates the endothermic process of iron oxide reduction with H<sub>2</sub>. Figure 6 illustrates the effects of microwave heating on the distributions of burden temperature (Figure 6a) and reduction degree (Figure 6b). In comparison with Case 2, the simulation referred to as Case 4 in the figure corresponds to a scenario with  $E_{mw} = 1.4$  MW. It is observed that the use of microwave heating gives rise to a general increase in both burden temperature and reduction degree, thus confirming the positive effect of microwave heating on the performance of the furnace. However, in evaluating the results, one should keep in mind the limitations imposed by the one-dimensional approach used in the present study.



**Figure 6.** Effects of microwave heating (with  $E_{mw} = 1.4$  MW) on the distributions of solid temperature (**a**) and solid reduction degree (**b**).

More simulations were carried out to study the effects of microwave power ( $E_{mw}$ ). Figure 7 depicts how the top gas temperature (a), top gas utilization degree (b), DRI metallization degree (c) and furnace productivity per unit volume of reduction zone (d) vary with  $E_{mw}$ . All four performance indices are seen to improve with an increase in  $E_{mw}$  because more thermal energy can be absorbed by the solid phase, which is in turn beneficial for the process. It should be pointed out that for the simulation with  $E_{mw} = 4.2$  MW, here referred to as Case 5, the productivity (32.4 t-Fe/(d·m<sup>3</sup>)) is nearly identical to that of Case 3 (with a 250 Nm<sup>3</sup>/t-pellet increase in  $G_H$ ). However, the increase in  $G_H$  requires a higher heating energy, about 6.8 MW, which indicates the promising energy-saving potential by using microwave heating.



**Figure 7.** Effects of microwave heating power ( $E_{mw}$ ) on predicted performance indices: top gas temperature (**a**), top gas utilization degree (**b**), DRI metallization degree (**c**) and productivity (**d**).

The thermochemical state in the furnace for the scenario of Case 5 can be studied in Figure 8, where the H<sub>2</sub> mole fraction of the gas phase (dash-double dotted line) and the equilibrium values of each reduction step calculated based on the solid temperature are plotted. As can be seen, the mole fraction of H<sub>2</sub> in the gas phase decreases as the stock-line is approached, while the equilibrium fractions increase. The differences between the curve for the mole fraction of H<sub>2</sub> in the gas phase and the curves for the equilibrium mole fractions represent the driving forces of the reduction reaction steps. It is seen that the wustite (Fe<sub>x</sub>O) reduction reaction, which is thermodynamically the most difficult step, takes place in the lower two thirds of the bed (H > 1.6 m), and its driving force increases as the lower-row injection point is approached.



**Figure 8.** Comparisons between mole fraction of H<sub>2</sub> remaining in the gas phase and the equilibrium values of each reduction step for the scenario of Case 5.

In order to shed more light on the conditions of Case 3 and Case 5, some indices of practical interest are listed in Table 4, where the top gas temperature for Case 5 is seen to be lower than the one for Case 3. This implies that Case 5 has a better utilization of thermal energy and thus a lower energy demand. The last row of Table 4 shows that the total (specific) energy demand for Case 5 is reduced by 0.2 GJ/t-Fe compared to the one for Case 3. Assuming that the price of electricity is 100 EUR/MWh, this energy saving corresponds to a reduction of 5.6 EUR/t-Fe in the production cost for the H<sub>2</sub>-based steelmaking chain essentially running on electricity. Moreover, the energy saving is equivalent to a decrease of 6.8 kg-coal/t-Fe in the fuel rate for the conventional coal-based steelmaking route, assuming the heating value of standard coal is 29.3 MJ/kg.

Index	Case 3	Case 5
Top gas temperature, K	718	690
Electrolysis energy, GJ/t-Fe	10.6	10.6
Heating energy, GJ/t-Fe	3.6	3.4
Compression energy, GJ/t-Fe	0.6	0.4
Microwave power, GJ/t-Fe	0	0.2
Total energy demand, GJ/t-Fe	14.8	14.6

Table 4. Predicted performance indices of two cases studied in this work.

## 4. Conclusions and Future Prospects

In this study, a mathematical model based on a description of the complex gas–solid countercurrent reactive flow was applied to investigate the performance of a shaft furnace for hydrogen reduction of iron oxide pellets under operation with a dual-row injection top gas recycling system. In addition, the potential of microwave heating was assessed briefly. The main findings of the study can be summarized as:

1. For scenarios without microwave heating, increasing the upper-row injection rate can improve the furnace performance, particularly in terms of top gas utilization

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degree and metallization degree of the direct reduced iron (DRI). Increasing the distance of the upper-row injection level from the furnace top also has a positive effect. However, at a critical value (around 3.5 m from the top under the operating conditions considered), a further increase tends to be ineffective for improving the performance. Moreover, it is expected to be most beneficial to apply microwave heating in regions above the upper-row injection level, where little metallic iron, which reflects microwaves, is present in the burden.

- 2. For scenarios with microwave heating, a higher microwave power generally gives rise to a better furnace performance in terms of top gas temperature, top gas utilization degree, DRI metallization and furnace productivity.
- 3. A high furnace productivity can be achieved by increasing either the upper-row injection rate or the microwave power. However, the total energy demand of the latter operation decreases due to a better utilization of thermal energy. Based on the comparison of two representative cases, the decrease in the total energy demand is about 0.2 GJ/t-Fe.

Even though the potential of the new design combining gas injection on dual levels and microwave heating was found promising, it should be kept in mind that the present analysis was based on a number of gross simplifications that need to be verified or revised. For instance, the thermal and reduction behavior of the burden under the condition of microwave heating should be investigated thoroughly in order to describe the impact more accurately. This concerns both the absorption of the microwave (i.e., the energy source in Equation (3)) and the effect of microwave heating on the reaction kinetics. In conjunction with this, the kinetic parameters describing the reduction of a single pellet in Equation (2) should be revised in order to better reflect the conditions in the H<sub>2</sub>-SF. Therefore, laboratoryscale experiments of the thermal and reduction behavior of iron oxide pellets under the conditions should be undertaken to develop sub-models of higher accuracy, which would improve the reliability of the predictions by the shaft model. Realizing the limitation of the one-dimensional approach taken in the present study, an extension to a three-dimensional model based on computational fluid dynamics is underway. This will make it possible to consider radial distributions of the state variables such as temperatures of the gas and solid phases, species fraction of the gas phase, reduction degree of the solid phase and possible asymmetry in the furnace. This will then make it possible to evaluate the penetration of microwaves and the gas injected at the upper row. Furthermore, a thorough study will be undertaken to assess the economic performance of the H<sub>2</sub>-based steelmaking chain, as well as a lifecycle assessment to evaluate the sustainability of this alternative ironmaking process.

**Author Contributions:** Conceptualization, Z.Z. and H.S.; literature review, S.Y., L.S. and H.S.; original draft preparation, S.Y. and L.S.; writing—review and editing, S.Y., L.S., Z.Z. and H.S.; funding acquisition, H.S. All authors have read and agreed to the published version of the manuscript.

**Funding:** This research was partially funded by Business Finland and companies in the project Towards Fossil-free Steel. The authors wish to express their gratitude for the financial support.

**Conflicts of Interest:** The authors declare no conflict of interest. The funders had no role in the design of the study or interpretation of the results.

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