Modelling and simulation of hydrogen reduction of iron ore in a direct reduction furnace

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Highlights

- Ironmaking processes cause huge emissions and must decarbonized in the future
- Computational study of hydrogen-based ironmaking in one and two dimensions
- Change from CO to H_2 as reductant strongly influences the thermal conditions
- Numerical simulation can guide the development towards more sustainable processes

1. Introduction

The steel industry is facing enormous challenges because of its large environmental impact: being largely coal-based today, iron- and steelmaking contribute by about 7% of the global CO_2 emissions [1]. The means to further suppress emissions in the presently dominating blast furnace-basic oxygen furnace (BF-BOF) route are strongly limited, because the BF cannot operate without coke as this material plays a structural role in the burden bed. The low-emission steelmaking option of most promise is the direct reduction (DR) process, where the iron ores would be reduced in solid state by hydrogen in shaft furnaces, producing direct reduced iron (DRI). The DR process is well established, but it is today operates on reformed natural gas, and it contributes by a small (6-7%) share of the world's iron production. The fully hydrogen-based counterpart is not yet operated in industrial scale, but scale-up is ongoing from pilot or demonstration units [2,3]. The aim of the present presentation is to shed light on DR furnace operation in hydrogen-rich gas atmosphere by mathematical modelling and simulation.

2. Methods

The shaft furnace was modelled in one or two dimensions, discretizing the variables in the vertical (1D) and radial (2D) directions. The models consider heat and mass transfer and chemical reactions, with a single-interface shrinking core model considering the stepwise reduction from hematite (Fe_2O_3) through magnetite (Fe_3O_4) and wüstite (Fe_x, with $x = 0.95$) to metallic iron (Fe) in the pellets [4]. For cases with only hydrogen in the feed gas, H_2 and H_2O are the only gaseous components, while for the case with H_2 and CO in the feed gas, the gaseous components considered are H_2, H_2O, CO and CO_2. The boundary conditions are the pellet feed flow rate, temperature and composition at the furnace top, and the gas feed flow rate, temperature and composition at the point of gas injection. The arising differential equations are solved numerically by pertinent methods. For the 1D model the calculation time is a few minutes, while it for the 2D model is 30 min - 2 h, depending on the problem formulation.

3. Results and discussion

The performance of the DR furnace was studied under different conditions to gain an overall view of the potential of using pure hydrogen or very high concentrations of hydrogen in the feed gas. Figure 1 shows the solid and gas temperature and burden metallization degree along the height of the furnace (panel a) and the rate of the stepwise iron oxide reduction reactions (panel b) predicted by the 1D model: note that wüstite is not stable at temperatures below 850 K. Panels c and d show the effect of the feed gas temperature and the reduction zone height, respectively, on the H_2 content of the in-furnace gas.

As for predictions by the 2D model, Figure 2 shows the temperature (panel a) and Fe mass faction (panel b) the burden for half of the cross section (due to axial symmetry) of the shaft furnace for five cases, where the H_2:CO ratio in the feed gas is 80:20, 85:15, 90:10, 95:5 and 100:0 labelled Cases 1-5. It is obvious that including CO in the reducing gas improves the reduction and thermal conditions in the furnace, the reason being the higher heat capacity of CO compared to H_2 and the overall exothermal effect of iron oxide reduction by CO by contrast to the endothermal reduction by H_2.

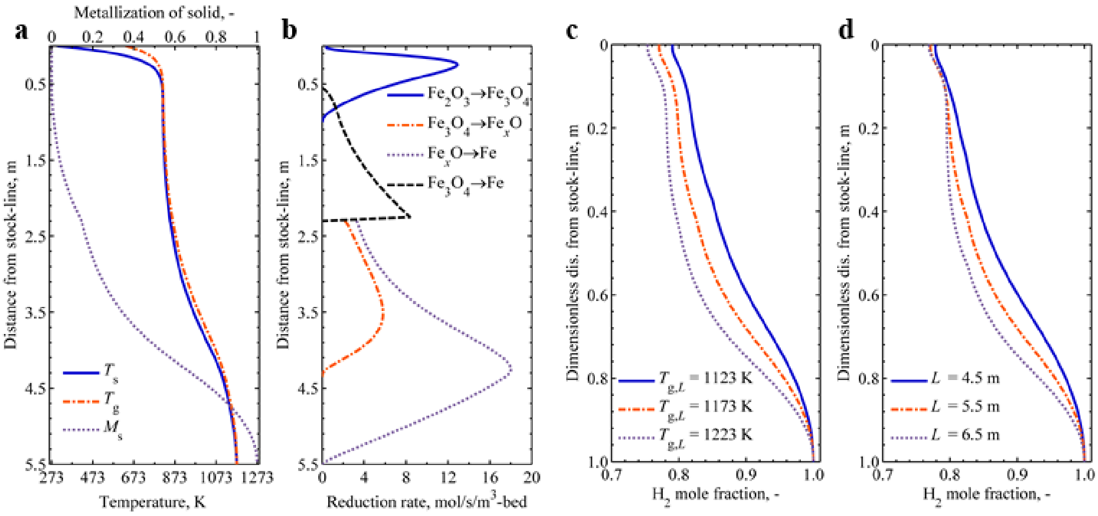

Figure 1. Results of 1D model: a) Gas and burden temperature and metallization degree, b) reduction reaction rates, c) effect of feed gas temperature, and d) reduction zone height on mole fraction of H_2 in the gas.

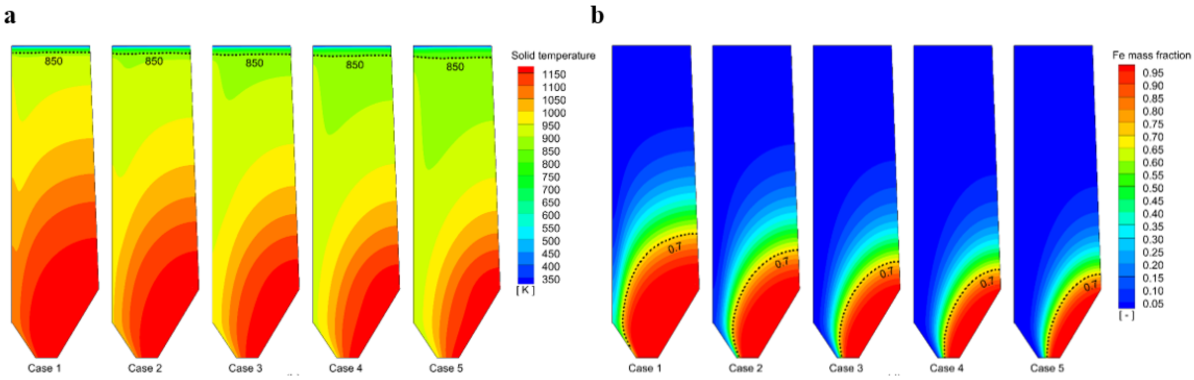

Figure 2. Results of 2D model: a) Burden temperature and b) Fe mass fraction distributions for different H_2:CO ratios in the feed gas.

4. Conclusions

The presentation has focused on a computational study of the potential to reduce the emissions in steelmaking by using hydrogen in a direct reduction furnace. 1D- and 2D-modeling has shed light on the internal conditions in the shaft furnace and has further clearly illustrated the impact of changing reductant from CO to H_2, and the consequences for the thermal state. The oral presentation will present more results and conclusions concerning the feasibility of the transition towards more sustainable steelmaking processes.

References

[1] IEA: https://www.iea.org/energy-system/industry/steel.
[2] HYBRIT: https://www.hybritdevelopment.se/en
[3] H2 Green Steel: https://www.h2greensteel.com
[4] L. Shao, Q. Wang, Y. Qu, H. Saxén, Z.-S. Zou, Metal. Mater. Trans. B 52 (2021) 451–459.

Keywords
Iron ore reduction; DRI furnace; simulation