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Direct iron reduction system analysis with mixture of hydrogen feed

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ABSTRACT

The present work explores computationally the potential of hybrid operation of a direct reduction shaft furnace with a feed gas mixture of methane and hydrogen, considering the operation of the associated gas handling and conversion units (reformers, condensers, heat exchangers, compressors, heaters, etc.). The state of the system is dependent on both the performance of the shaft furnace, which is sensitive to the feed gas composition and quantity, and the reformer, which converts the methane and the recycled top gas from the shaft furnace into feed gas. This coupling gives rise to nonlinear behavior of the system with respect to changes in the boundary conditions, which justifies a model-based approach for holistic analysis. The system is modelled in Aspen Plus to simulate the operation of an industrial-scale plant using a detailed model of the process units. Three configurations of the system are evaluated: (i) co-feeding of hydrogen with methane, (ii) feeding hydrogen directly to the shaft furnace, and (iii) splitting the hydrogen feed between the two injection points. Further, the effect of H_2 share in the feed was evaluated in terms of energy consumption, CO_2 emissions and energy cost with low- and relatively high-carbon electricity. The results show that increasing the share of hydrogen in the fresh feed leads to lower CO_2 emissions, considering low-carbon electricity.

Keywords: Hydrogen, Direct reduction, Steam reforming, CO2 emissions, Energy cost

INTRODUCTION

The iron- and steelmaking industry is the foremost source of industrial CO_2 emissions with a share of 27%, emitting 2.6 Gt/a in 2022 [1], [2]. The sector is particularly energy intensive accounting for 20% of global industrial energy demand, relying mostly on fossil sources. The global production of steel has almost doubled within the last two decades, creating an urgent need to accelerate the decarbonization of this sector [3]. Various pathways have been investigated for a green transition of iron and steel industries, relying on process efficiency and switching to alternative feedstocks and fuels with lower carbon footprints. A strong concept that has been explored is the replacement of blast furnaces, which rely heavily on coke and coal, by direct reduction shaft furnaces (SF) operating on hydrogen-rich gas mixtures. A full transition to hydrogen-based iron ore reduction is a promising pathway to limit the carbon footprint. However, there are still challenges that hinder its adoption by steelmakers, notably the endothermic nature of the reduction reactions, the lower heat capacity of the gas, and, foremost, the high price of green hydrogen. Recent studies have indicated that it may be beneficial to include some carbon monoxide in the feed gas due to its positive impact on the heat supply and less endothermic reduction reactions [4].

The MIDREX process is one primarily gas-based technology for direct reduction of iron ore, representing about 80% of SF-based global steel production [5]. To support the transition toward H_2-based reduction, the MIDREX-flex process offers flexible operation using both natural gas (NG) and H_2, allowing a smooth and controllable transition for steelmakers [6]. It also enables the retrofitting of existing plants rather than requiring a complete redesign. However, the process behavior during this transition is not clearly known as most of the research works evaluate a complete transition to H_2.

The current study evaluates computationally the operation of an iron ore direct reduction process with top gas recycling by gas handling and conversion units

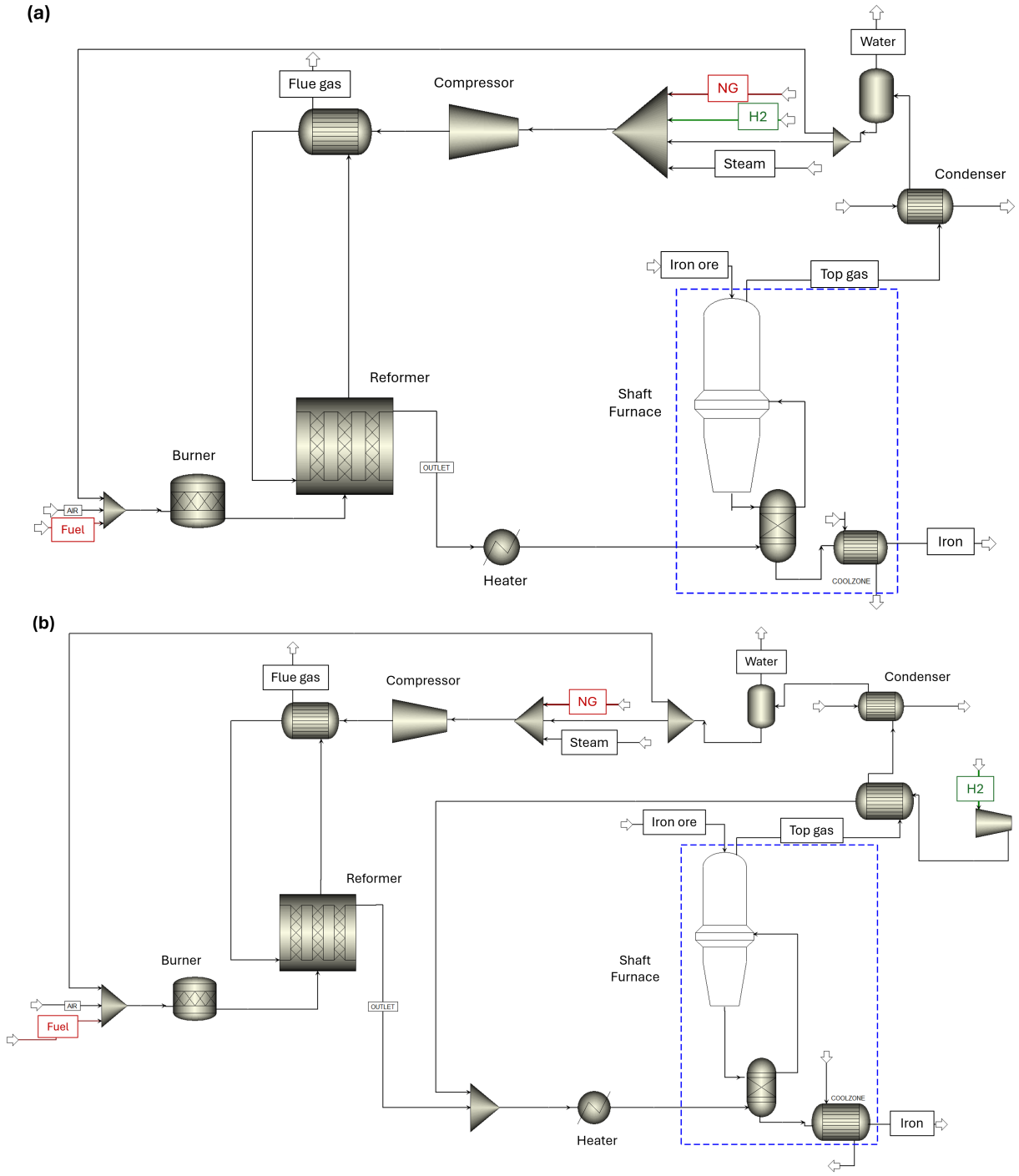

Figure 1. Process flowsheet of the direct reduction process.

(reformers, condensers, heat exchangers, compressors, heaters, etc.). The process operation is studied under varied shares of H_2 in the feed with different possible injection points in the system. Fresh gas and fuel demands, energy consumption and costs are analysed along with the total CO_2 emissions. The study provides guidelines for possible future operation states of iron direct reduction.

METHODOLOGY

Process description

The current work considers a shaft furnace

Table 1: Process and fuel gas consumption for the evaluated cases.

Description	**Case 1** H_2 injection at reformer upstream	**Case 2** H_2 injection at SF level	**Case 3** H_2 injection split at reformer upstream and SF inlet	**Case 4** Only H_2 based reduction	**Case 5** Only CH_4 based reduction
H_2 feed (kNm^3/h)		27.11		80.69	—
CH_4 feed (kNm^3/h)			22.09		31.38
Fuel consumption (kNm^3/h)		56.03		—	56.03

employing rich gas mixtures for the iron ore reduction. The process operates with both H_2 and NG, where H_2 represents 55 mol% of the combined feed. The shaft furnace top gas is recycled back to the system after water removal and mixing with the fresh feed. The process gas is compressed and preheated before entering a steam methane reformer (SMR) for converting CH_4 into a rich mixture of H_2 and CO, in the presence of recycled top gas. An electric heater is included for further heating of the syngas. It is important to note that 70% of the SF top gas is recycled as process gas, while the other part is fed to the reformer burner along with fuel gas (NG). **Figure 1 (a)** illustrates the process layout of the base case scenario, where both H_2 and NG are fed to the reformer.

The paper investigates two other cases with different injection points of H_2. The second case assesses the scenario where H_2 is supplied directly at the inlet of the SF after being preheated by the top gas, as represented by **Figure 1 (b)**. In the third case, the H_2 feed is split so that half of it is fed with the NG and the other half is supplied at the SF inlet. Fully H_2-based and CH_4-based direct reduction scenarios are considered as reference cases, corresponding to cases 4 and 5, respectively. **Table 1** summarizes the cases with H_2, CH_4, and fuel consumptions.

It is worth mentioning that the feed of H_2 and CH_4 is kept constant for the three first cases, while for cases 4 and 5 it is varied to achieve a production of 100 t_{DRI}/h with a metallization rate of 0.93, which is the target production for all the cases.

Model framework

Reformer model

The system is modeled using Aspen Plus software (V14). First, the model of the SMR is a plug flow reactor with co-current thermal fluid to simulate an industrial reformer with multi-tubular reactor geometry. The reactor catalytic tubes have a length of 7.9 m, with an internal diameter of 0.2 m [7], and a heat transfer coefficient estimated as 750 W/m^2 K [8]. The Peng-Robinson thermodynamic model is used for mass and energy balances of the system, while the pressure drop throughout the reformer is estimated using the Ergun equation.

The main chemical reactions occurring are the steam methane reforming reaction (Eq. (1)) and the water-gas-shift reaction (Eq. (2)):

$$CH_4 + H_2O \rightleftharpoons CO + 3H_2 \; \Delta H_{298\,K} = 206.1\; kJ/mol \quad (1)$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \; \Delta H_{298\,K} = -41.15\; kJ/mol \quad (2)$$

The reactions kinetics over nickel-alumina catalysts have been widely investigated in literature [9], [10], [11]. The Langmuir-Hinshelwood-Hougen-Watson (LHHW) model is employed to determine the reaction rates, as an accurate model that considers surface reactions making it suitable for modelling catalyst-based processes [12], such as methane reforming.

Shaft furnace model

A one-dimensional open source steady-state model, developed by Aspen Technology [13], is used to simulate the SF. The model was implemented in Aspen Custom Modeler (ACM), modeling a counter-current flow of descending iron ore pellets and ascending reducing gases. An RGibbs reactor is integrated to simulate the water-gas-shift and methane reforming reactions over an iron oxide catalyst, and a heat exchange is employed for cooling down the metallized iron to 100 °C. The key reactions for the direct reduction can be expressed as follows:

$$Fe_2O_3 + 3H_2 \longrightarrow 2Fe + 3H_2O \quad (3)$$

$$Fe_2O_3 + 3CO \longrightarrow 2Fe + 3CO_2 \quad (4)$$

The evaluation of energy consumption considers the required compression power, heating duty, and H_2 production via electrolysis. Total carbon dioxide emissions are investigated by accounting the emissions linked to process electricity consumption in addition to the

direct emissions with flue gases. Finnish and EU average energy and emissions contexts are used for the analysis.

SIMULATION RESULTS

Effect of hydrogen feed point

To find optimal operation points of the direct reduction process, the possible injection points of hydrogen are evaluated as described in **Table 1**. The system behavior is analysed in terms of the metallization rate of direct reduced iron (DRI), energy consumption, and total CO_2 emissions.

Table 2 lists the energy consumption of the process in terms of electricity consumption (EC) and primary energy consumption (PEC). Comparing the three injection points of H_2 (Cases 1—3), the first scenario, where hydrogen is co-fed with methane, enables the least energy consumption. This is because less heating is required at the inlet of the SF to maintain syngas temperature at 940 °C. The process gas exits the reformer with relatively high temperature (around 850 °C). Thus, the heater needs to provide a limited temperature increase, whereas the alternative injection options involve cooler gas entering the heater and therefore increasing the heating duty. On the other hand, it is observed that H_2-based direct reduction requires higher energy input, most of it in the form of electricity, with a large share for powering the electrolyser (83%).

Table 2: Electricity and primary energy consumption of the system in different scenarios.

	PEC (MW)	EC (MW)
Case 1	549.8	160.9
Case 2	553.3	163.8
Case 3	551.6	162.4
Case 4	647.1	471.5
Case 5	406.9	32.5

With regards to the syngas composition, it is found that the injection point of H_2 does not have a significant effect on the molar composition. In the current steady-state model, the feed of H_2 and CH_4 is similar for the three cases, in addition to the fuel consumption that permits a CH_4 conversion around 0.9. Thus, the overall mass balance of the system remains nearly unchanged.

Figure 2 represents the total CO_2 emissions of the system considering (a) Finnish and (b) EU average contexts. The grid emission factors used for the study are 29.5 and 187 gCO_2/kWh, respectively, based on the statistics of 2024 ([14], [15]). With regards to the different scenarios (cf. **Table 1**), direct emissions are the major contributor to total CO_2 emissions, considering the current share of H_2 in the system. Further, H_2-based direct reduction enables total emissions abatement in the order of 81%, compared with methane-based reduction process, in the Finnish context. However, the emissions of hydrogen-based system rose to surpass the conventional system (case 5) by 12% in the average EU context. Therefore, the hybrid and hydrogen-based processes are environmentally attractive only when electricity has lower carbon footprint and a higher part of renewables.

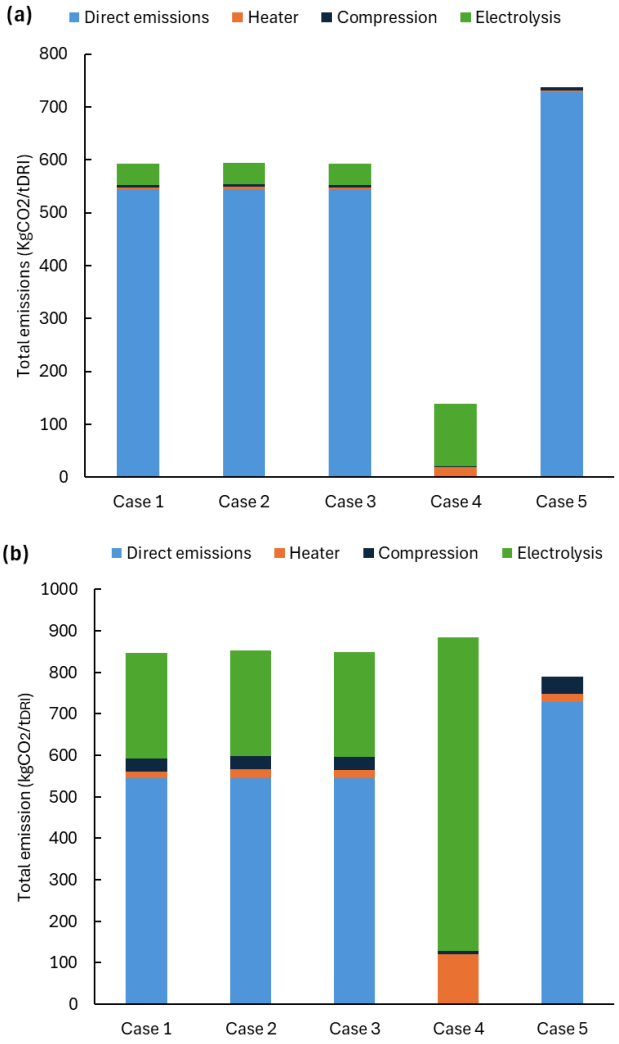

Figure 2. Total emissions of the system under different scenarios for (a) Finnish and (b) EU average contexts.

The analysis of energy cost shows that the reduction route combining H_2 and CH_4 results in a 5% cost reduction, compared with CH_4 based DRI process, while the fully hydrogen-based route allows 32% of energy cost reduction, in the Finnish scenario (**Table 3**). In contrast, for the average EU context, the energy cost was increased by 1.6 to 3 folds, comparing with the conventional system, due to higher electricity consumption.

Table 3: Energy cost under different scenarios (€/t_{DRI})

	Finland	EU average
Case 1	300.8	348
Case 2	302.2	352.1
Case 3	301.5	350.1
Case 4	217.4	652.2
Case 5	317.7	212.5

Effect of hydrogen share in the feed

To evaluate the process behavior under different shares of H_2, **Figure 3** illustrates the variation of energy consumption and CO_2 emissions. It is observed that as hydrogen share increases in the fresh feed, the energy consumption increases as well, because of increased electricity demand. Total emissions of the system decrease with higher shares of hydrogen, caused mainly by lower direct emissions. Note that the Finnish context is considered in this part of the study.

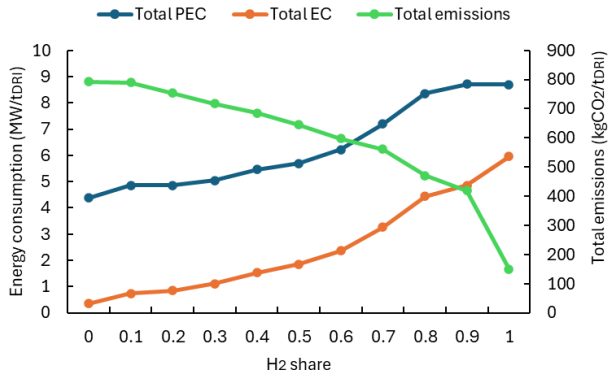

Figure 3. Effect of H_2 share on energy consumption and CO_2 emissions.

Figure 4 shows the variation of energy cost with the hydrogen share in the feed. Following the increase of electricity consumption, the electricity cost rises linearly with the H_2 part. At low to moderate H_2 shares (up to 0.7), the cost of NG, used as reducing agent and fuel, is the primary driver for the energy cost. In these cases the process relies significantly on NG to achieve the desired iron ore reduction rate while the cost of NG in Finland is relatively high [16]. Therefore, the transition to hydrogen-based direct reduction is economically wise in regions where electricity is cheaper. Total energy cost remains approximately constant over a wide range of hydrogen shares, as the savings in NG cost are offset by the rising electricity demand.

It is worth mentioning that more in-depth economic analysis is required to assess the feasibility of the green transition, accounting for investment costs in addition to operational costs.

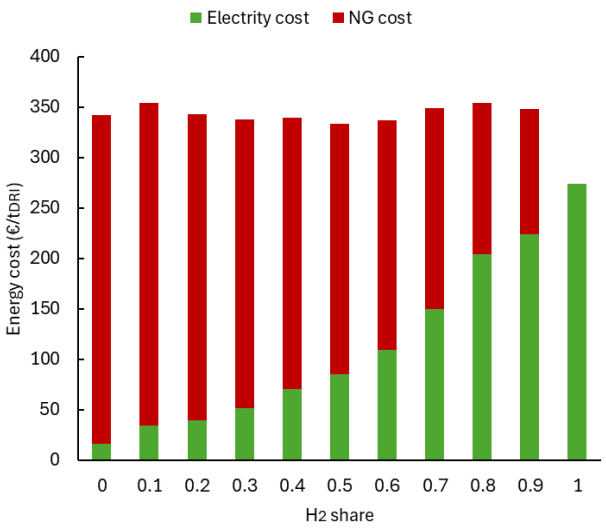

Figure 4. Effect of H_2 share on energy cost.

CONCLUSION

The present work investigates a process for direct reduction of iron using a mixture of methane and hydrogen. The system includes steam methane reforming and a direct reduction shaft furnace in addition to heat exchangers, a condenser, and a heater, which are modeled using Aspen Plus software. The effect of having different hydrogen injection points in the process was evaluated, along with the variation of H_2 share in the fresh gas feed. Energy consumption, total emissions, and energy cost are the key performance indicators employed to evaluate the process.

The results outline that the feeding point of hydrogen in the system has a negligible impact under steady state mode. However, co-feeding hydrogen with methane is favored for its relatively lower energy consumption. Evaluating the total CO_2 emissions shows that a hybrid route for direct reduction can reduce 25% of the emissions compared with fully methane-based reduction. Further, the carbon intensity of electricity is a critical determinant of overall system emissions; up to 97% of CO_2 can be avoided when low-carbon electricity is available, whereas a high-carbon electricity supply can limit these benefits and even lead to higher emissions than the conventional reference case. On the other hand, increasing the hydrogen part in the fresh feed leads to lower total emissions when low-carbon electricity is available. From an energy cost perspective, it is found that hydrogen-based direct reduction is economically wise. However, a more in-depth economic study is necessary to identify the cost effectiveness of the system.

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