

CFD Study of an Energiron Reactor Fed With Different Concentrations of Hydrogen



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Climate change is one of the defining challenges of our era and the iron and steel sector is responsible for approximately 7% of global CO₂ emissions. Innovative hydrogen-based technologies are being developed to decrease the carbon footprint of tomorrow's steelmaking plants. In this context, Energiron is a mature direct reduction technology that maximizes the efficient use of hydrogen for direct reduced iron (DRI) production. This paper presents a computational fluid dynamics analysis of an Energiron reactor operating with different levels of hydrogen; the resulting momentum, species and enthalpy balances for both the DRI and the gas phases are described and analyzed.

Iron and steel production is a fundamental sector for the growth and development of a country. The industrial world produces around one-quarter of global gross domestic product (GDP) and employment, making it possible to procure all those materials and goods that people need every day, so it can be understood how this sector plays an important role in everyday life. Nonetheless, industry accounts for up to 28% of the world's greenhouse gas (GHG) emissions and iron- and steelmaking have the lion's share of that percentage, with a quota of emissions that is around ⁷/₈ of the total. However, steel has an advantage compared to other materials: it is 100% recyclable, which makes it the perfect material to guarantee a circular economy and thus make the world more sustainable.

Furthermore, the world's steel demand is constantly growing, and the forecast for 2050 is that annual steel consumption will be in the range of 2.6 billion tons. In order to meet these demands in a sustainable way, it is necessary that steel production be shifted toward technologies that provide the same quality and throughput while reducing CO₂ emissions.

The electric arc furnace (EAF) route is fed by scrap or hot briquetted iron (HBI)/direct reduced iron (DRI), so the carbon footprint is lower. However, scrap supply is

limited, particularly in emerging countries, and new iron sources for crude steel production need to be introduced in the market. World iron production relies on mainly the blast furnace (BF), which has the larger share, while DRI covers a smaller part. The BF route is already fully optimized; therefore, no CO₂ reduction can be achieved without major process modifications. The addition of scrap or DRI to increase production and decrease CO₂ emissions was suggested for the BF route, but these are not primary sources, thus it is not a solution. Hydrogen enrichment in blast furnaces encountered some problems during operation and should be limited,¹ so the hydrogen route is not an option for the BF. The most promising technology would require a blast fed by pure O₂ to ease CO/CO₂ separation from the top gas and CO recycling in the BF itself (top gas recycling or TGR). Furthermore, green electric energy would be required for O₂ production to avoid further CO₂ emissions. TGR is not something that can be applied gradually and would reduce carbon footprint by 25%; thus the need for considerable investments, green electric energy, and suitable carbon capture and storage (CCS) technologies for the remaining 75% of CO₂ means that this solution cannot be applied yet. If the industry does not want to rely on CCS technologies, which

probably don't have the capacity to cope with the steel industry's CO₂ production, there needs to be a shift toward a pure electric or pure H₂ route, moving from carbon capture to carbon avoidance. Pure electric processes have low technology readiness levels (TRLs) and could only be considered in the future. Now the most convincing and ready technology is hydrogen-based direct reduction.

A Solution for Direct Carbon Avoidance — The Energiron Zero Reformer (ZR) technology is already known to be able to reduce the carbon footprint of ironmaking thanks to the use of natural gas as a reducing gas (instead of the coking coal used in integrated steel works). In general, every Energiron process is characterized by the intrinsic removal of CO₂ from the recycled gas.

This second point alone renders the technology able to selectively remove about 60% of its CO₂ emissions, which can then be stored or destined for other uses, whenever these solutions are available. Since the basic process scheme (depicted in Fig. 1) is the

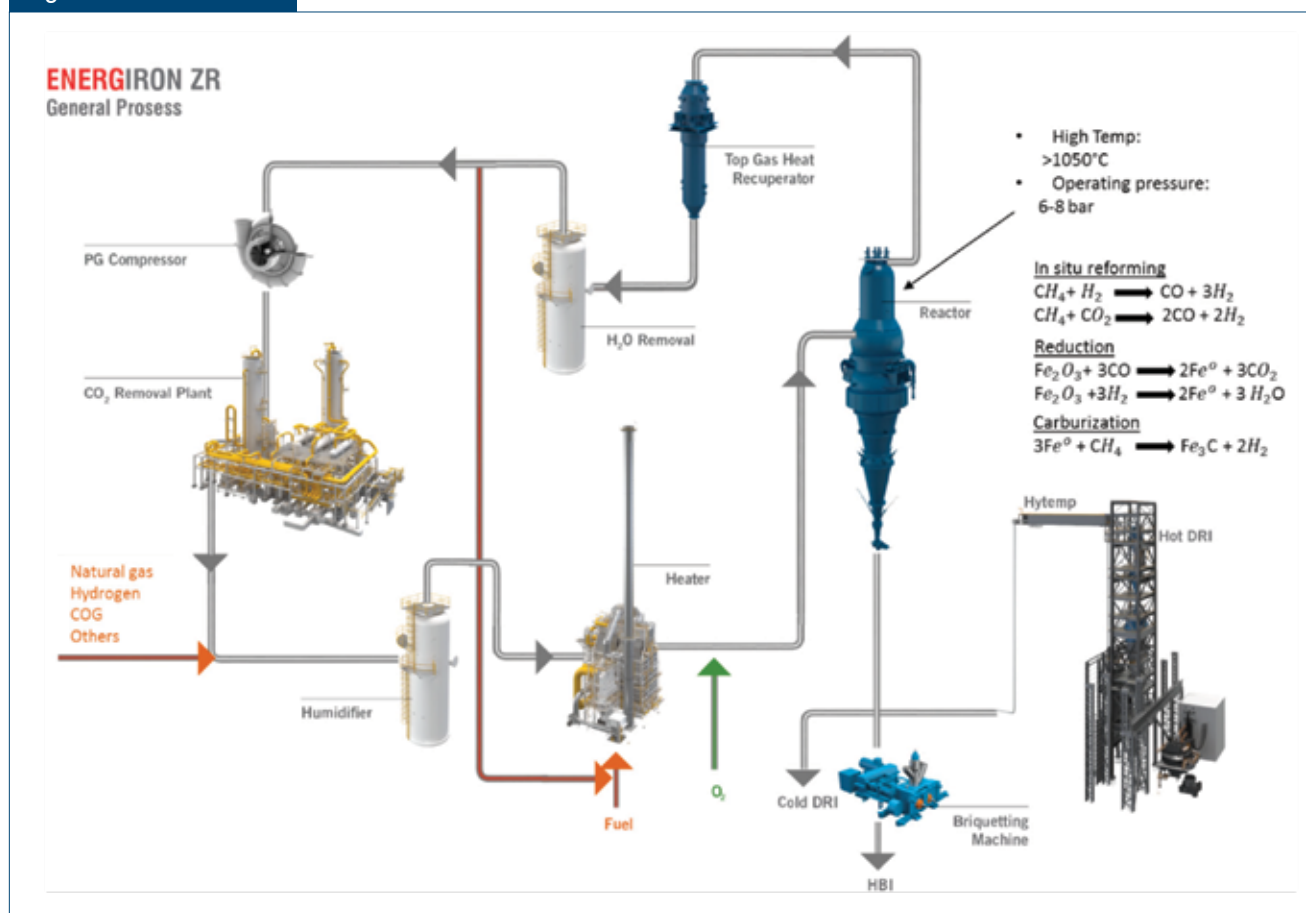
same regardless of the nature of the makeup gas, if there are users for the separated CO₂, Energiron can reduce CO₂ emissions even when using reducing gases with less “green” characteristics, e.g., coke oven gas or syngas from coal gasification.

Switching to a feed gas made of hydrogen only would be the real game-changer, because it would completely avoid the generation of carbon dioxide from the process, since the only product of reduction reactions would be H₂O.

Energiron plants are already running with high H₂ content in the reducing gas; as a matter of fact, the typical H₂/CO ratio for an Energiron ZR plant is around 3 ÷ 4, while in an Energiron plant with an external reformer this value can increase to 4 ÷ 5.

This shows that an Energiron plant is capable of handling high hydrogen content (virtually up to 100%) without major changes to its equipment, and it is a technology which is a step ahead toward a sustainable ironmaking future, rendering carbon direct avoidance a reality. The study presented in this paper will also show, via computational fluid dynamics

Figure 1



Basic scheme of the Energiron direct reduction process.

(CFD) simulations, that the increase of hydrogen content in the entry reducing gas does not affect the reactor's behavior, guaranteeing high metallization in all cases.

Fluid Dynamic Modeling

Previous Studies: Numerical simulations are valuable tools in the field of research and development. Complex interactions among gas and solid fluid dynamics, thermal fluxes and chemical reactions can be implemented in a single model that offers an overview of the whole industrial process. Several simulations and studies on direct reduction reactors, attempting to describe the reduction process, have been performed in both 1D and 3D.²⁻⁸

A previous study demonstrated the possibility to closely predict the solid flow field, comprising its internal stresses, and to calculate the flow field of the gas flowing through the porous bed, together with the thermal and chemical description of both solid and gas phases.¹⁰ The model was able to reproduce the behavior of an industrial direct reduction process (DRP) reactor operated at high pressure, in terms of product metallization and total carbon content of DRI. Moreover, the model was capable of simulating two very different reactor configurations without the need to change any model parameters: reducing gas produced by an external reformer or direct injection of natural gas into the process (the ZR configuration) are equally well represented in the model.

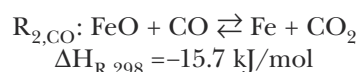
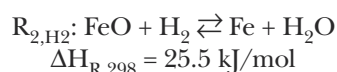
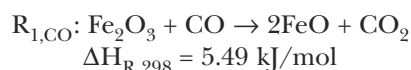
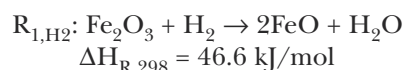
This study is based on a previous one and goes into more detail on makeup gas composition with three different feeds, showing the related metallization, carbon and temperature maps.

Model Overview: Solid flow is treated as a non-Newtonian continuum fluid. The proposed rheology provides the closure of the model by describing the effects of pellet velocity fluctuations on viscosity, with a kinetics-based mathematical model. Boundary conditions at the wall implement a “slip length” that reproduces the interactions between the solid and the wall (the typical slip-stick motion of granular materials). Moreover, solid phase continuity must account for mass transfer between solid and gas phases due to carbon deposition and reduction reactions, respectively.

Gas continuity is described by mass balances based on solid continuity; therefore, the mass variation of the gas phase will be the same in value but with an opposite sign to that of the mass variation of the solid phase. Therefore, the whole system (gas+solid) correctly shows global mass continuity. The gas momentum equation contains both viscous and inertial dissipation terms, in accordance with the Brinkman-Forchheimer equation.

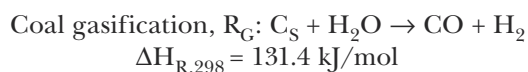
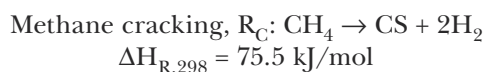
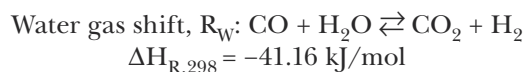
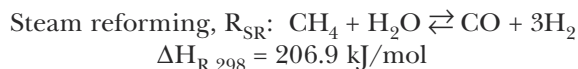
Species and energy balances are calculated in more detail both for the gas and the solid phase, including convection, diffusion and reaction terms. A more detailed description can be found in Reference 9.

Kinetic Model: The reduction of iron ore involves heterogeneous reactions between solid and gas species. Iron ore, mainly constituted by hematite (Fe_2O_3), is gradually reduced to magnetite (Fe_3O_4), wüstite (FeO) and iron (Fe). The ore contains some gangue (SiO_2 , CaO , etc.) as well, which is assumed to be an inert substance in the reduction process. Since the reaction from hematite to magnetite is very fast compared to wüstite reduction — only the steps from hematite to wüstite and from wüstite to iron are considered — each of them with both hydrogen and carbon monoxide. Reactions from wüstite to iron are considered reversible and linked to the thermodynamic equilibrium FeO/Fe .



The functional form of the reaction rate is based on the shrinking core model, in which reagents have to pass through one or more layers of products, from the outside to the inside of the pellet, before reaching one of the chemical interfaces: hematite-wüstite or wüstite-iron.

Besides the reducing ones, there are other reactions taking place inside the reactor, catalyzed by metallic iron and involving the gas species.



All the kinetic rates of the reduction and the catalytic reactions are multiplied by a factor δ that describes the deceleration of the kinetics due to carbon deposition,

very well documented by Reference 10. The main effect of carbon is to add a further diffusive resistance because iron is well known to enhance the formation of carbon nanotubes,¹¹ which plug the inner porosity of the pellets, hindering both reduction and catalytic reactions. The critical mole fraction at which carbon starts limiting the process, here called y_C^* , is linked to the solubility of carbon in iron, thus the critical mole fraction depends on temperature according to the Fe-C diagram.

Discussion

The plant considered in this paper is a 2.5 MPTY Energiron ZR plant (321.5 th), producing HBI with a 94% metallization degree.

For the study, three distinct feeds were considered:

- 100% natural gas (NG).
- 50% natural gas/50% hydrogen (on an energy basis).
- 80% hydrogen/20% natural gas (on an energy basis).

Carbon content of the product depends on the percentage of natural gas in the feed mix, since NG is the only source of carbon added to the process. It can vary from 0.6% in the 80% H₂ case to 1.5% in the 100% NG case.

The feed mixes stated before are related to process only; the open flames of the plant (like process gas heater burners, pilot flames and so on) are considered

to be fed by a mixture of natural gas and tail gas from the process in every case.

The natural gas used in simulations has a 91% content of CH₄, 5.6% of C₂₊, 1.75% nitrogen and the rest CO₂. Hydrogen, on the other hand, is considered to be 100% H₂.

Case 1: Natural Gas Feed — In this scenario, the process scheme is the Energiron ZR (Fig. 2). Natural gas is added to recycled gas after CO₂ removal and the mixture of these two streams is sent to the humidifier (to control H₂O content) and to the process gas heater, where it is heated to about 950°C. Oxygen injection helps increase bustle gas temperature to 1,100°C before it enters the reduction reactor.

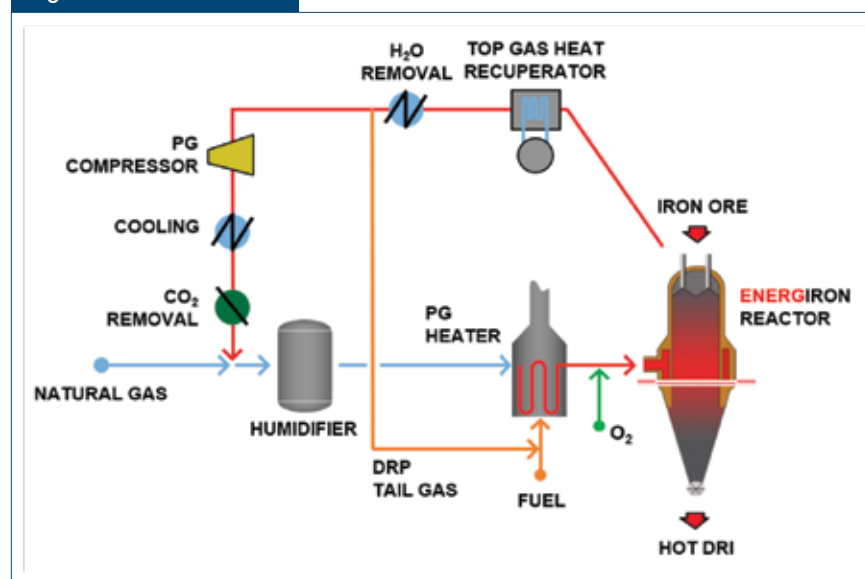
Spent gas leaving the top of the reactor is first passed through the top gas heat recuperator (to exploit residual sensible heat), then it is cleaned of dust and cooled to separate reduction products such as H₂O and CO₂. After this last step, the recycled gas is ready to be mixed with natural gas and enters the cycle again.

In this configuration, the composition of the bustle gas entering the reactor is as per Table 1. The required flow of bustle gas at reactor inlet is around 670,000 Nm³/hour.

This process scheme has a specific consumption of 2.34 Gcal/t, corresponding to 266 Nm³/metric ton of natural gas, and the resulting HBI has 1.5% of carbon. In addition to chemical energy consumption, electrical energy consumption must also be considered, which in this case is 103 kWh/t.

CFD Simulation of Case 1 — Reducing gas enters the reactor radially from the bustle gas distributor, along the entire circumference. Thus, gradients of temperature and reducing gas composition exist in the inner volume of the reactor and this has an impact on the radial profiles of solids (Fig. 3). Metallization is almost complete at the periphery,

Figure 2



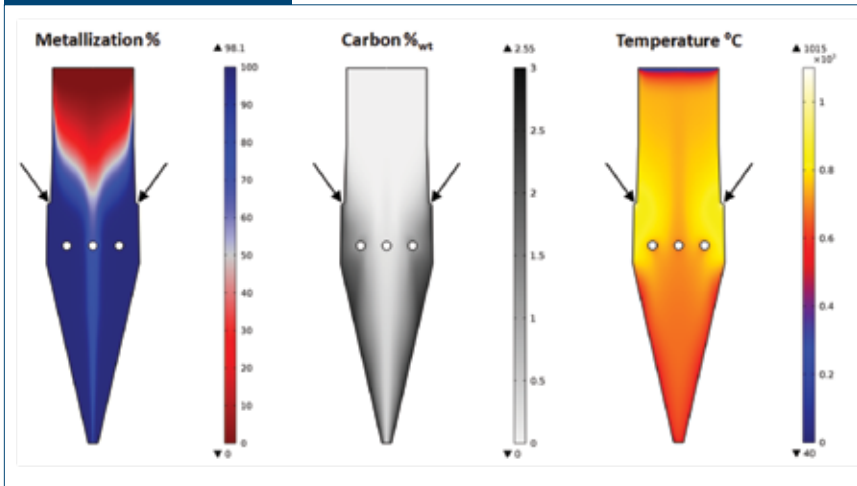
Classical Energiron ZR process scheme.

Table 1

Composition of Bustle Gas in Scenario 1

H ₂	[% vol.]	47.9%
CO	[% vol.]	14.8%
H ₂ O	[% vol.]	11.0%
CO ₂	[% vol.]	1.7%
CH ₄	[% vol.]	19.5%
N ₂	[% vol.]	5.1%

Figure 3



Results from Case 1: metallization, carbon and solid temperature maps.

where temperature and reductants are at their maximum levels, while it has a profile decreasing toward the center of the reactor, where only 1% of pellets have a metallization <88%. Calculated mean metallization is 94%.

Carbon deposition is catalyzed by metallic iron and favored at high temperature in the presence of hydrocarbons and hindered by oxidants, in particular steam; therefore, the carburation zone goes from the bustle gas injection point downward, where hot metallic iron meets the least oxidized hot reducing gas in countercurrent. Mean carbon content of DRI in this case is 1.5 wt.%.

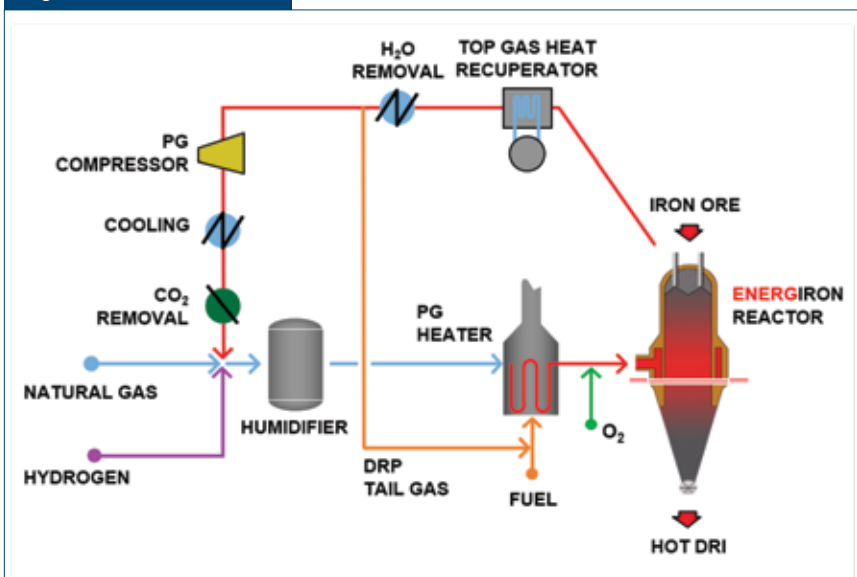
cone walls. Temperature discharge in Case 1 is around 700°C.

Case 2: 50% NG/50% Hydrogen Feed — In this case, the only modification to the process scheme is the addition of hydrogen as fresh feed to the recycled gas, just as it is done with natural gas. The relatively high content of natural gas in the feed mix (and therefore of carbon dioxide in the top gas) means that it is not possible to bypass equipment such as the CO₂ removal plant or the humidifier yet.

With the increased amount of hydrogen fed to the process, the bustle gas entering the reactor has the composition reported in Table 2. The flowrate of bustle gas entering the reactor is approximately 610,000 Nm³/hour.

The process under these conditions consumes 2.17 Gcal/metric ton of energy, corresponding to 156 Nm³/metric ton of natural gas and 308 Nm³/metric ton of hydrogen. In this case, due to the

Figure 4

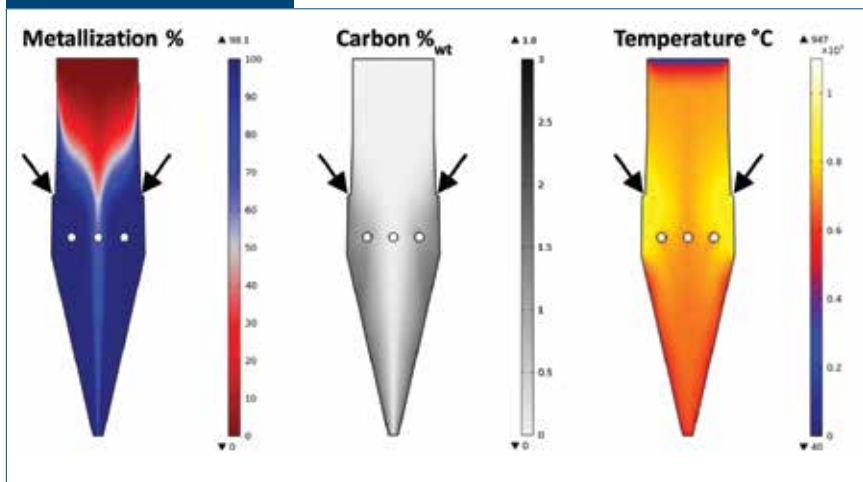


Process scheme with added hydrogen.

Table 2

Composition of Bustle Gas in Scenario 2		
H ₂	[% vol.]	63.4%
CO	[% vol.]	8.1%
H ₂ O	[% vol.]	4.7%
CO ₂	[% vol.]	0.4%
CH ₄	[% vol.]	16.5%
N ₂	[% vol.]	6.9%

Figure 5



Results from Case 2: metallization, carbon and temperature maps.

lower circulating volume of gas and thus lower compressor consumption, electrical energy consumption is 91 kWh/metric ton.

CFD Simulation of Case 2 — In Case 2, reactor performance is quite similar to Case 1 (Fig. 5). By replacing part of the natural gas with hydrogen, reactivity is enhanced and endothermicity is mitigated. As a consequence, process gas flow is reduced by 8% and inlet temperature is reduced by 115°C.

Mean metallization is always 94%, with a slightly more pronounced distribution curve. The carbon map is quite different from that in Case 1, because the lower carburizing potential produces a modest carbon deposition. Mean carbon in the product would be around 1%.

The temperature map is quite interesting for this case. Lower flowrate means lower convective heating, so the zone of ore pre-heating widens a little. Furthermore, temperature in the upper zone is somewhat lower than before, slowing down the reactions, which take place a little more downstream than before. On the contrary, due to the lower carburization achieved in the below-bustle zone, the temperature level in the cone is higher and product discharge temperature reaches 750°C.

Case 3: 80% Hydrogen/20% Natural Gas Feed — Increasing hydrogen feed more strongly reduces the

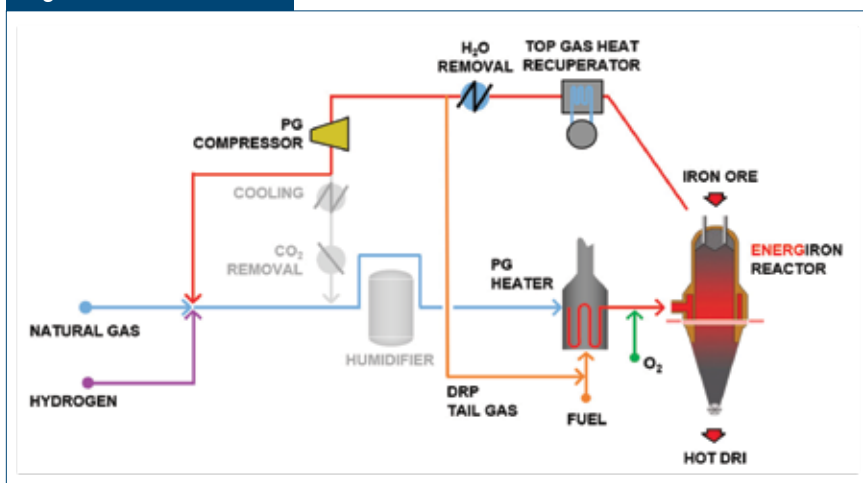
CO₂ content in the top gas, and therefore it is no longer necessary to separate it from the top gas before recycling it. The CO₂ removal plant could be bypassed under these circumstances, as well as the humidifier, due to the low hydrocarbon content of the feed gas (see Fig. 6).

As per Table 3, bustle gas composition is clearly hydrogen-oriented. The bustle gas flowrate is reduced even more than in Case 2, down to less than 590,000 Nm³/hour.

The total energy consumption of the process in Case 3 is 2.11 Gcal/metric ton, given by 106.5 Nm³/metric ton of NG and 455 Nm³/metric ton of hydrogen. In this case, electrical consumption is even lower — 86 kWh/metric ton.

CFD Simulation of Case 3 — Results of Case 3 are shown in Fig. 7. Because of a H₂ content higher than 70%, the process gas flowrate decreased by another 5% with respect to Case 1, and temperature by another 50°C. The

Figure 6



Process scheme with 80% hydrogen feed.

Table 3

Composition of Bustle Gas in Scenario 3

H ₂	[% vol.]	72.5%
CO	[% vol.]	4.7%
H ₂ O	[% vol.]	2.6%
CO ₂	[% vol.]	0.1%
CH ₄	[% vol.]	15.5%
N ₂	[% vol.]	4.6%

metallization map moves downward a little more while keeping a mean of 94% in the product. The carburization reaction is even more attenuated, thus carbon in the product is now 0.6%. Temperature inside the reactor follows the same trend as from Case 1 to Case 2, decreasing in the upper reactor but remaining quite high in the lower reactor, so that discharge temperature is still around 750°C.

Carbon Footprint — This section is dedicated to analyzing the carbon footprint of the different scenarios presented before. To perform this evaluation, some assumptions had to be made:

- The carbon footprint of the upstream plants (iron ore production, cement production, etc.) is not considered since it is the same for all cases.
- Hydrogen production via electrolysis is taken into account with a consumption of 56 kWhEE/kgH₂.
- A sensitivity analysis of the electrical energy footprint was performed, and it considered

20 gCO₂/kWh for green sources/nuclear, 490 gCO₂/kWh for electrical produced by gas and 820 gCO₂/kWh for electrical coming from coal.

- CO₂ emissions coming from the process and from heater fumes are calculated separately since process emissions are selectively removed and are available for CCS or other uses. They will be called selective and non-selective emissions.

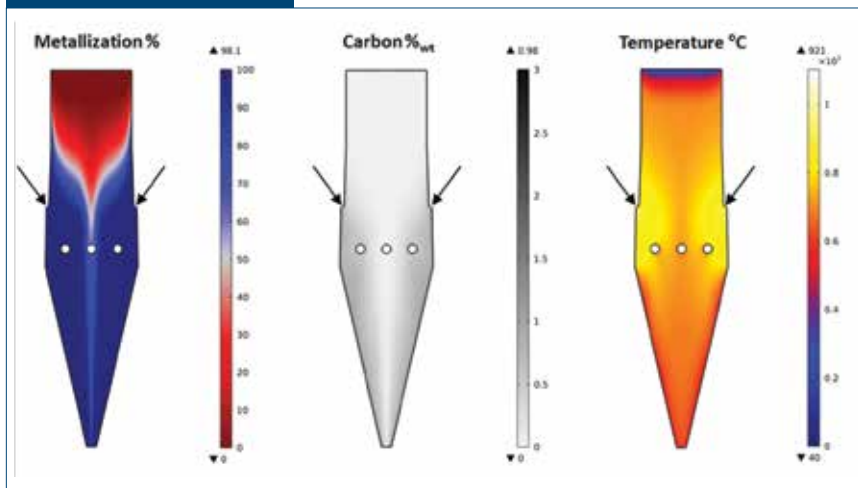
Under these assumptions, the carbon footprint of the different cases is reported in Table 4.

Hydrogen as a gas is not available on Earth; as a matter of fact, it is almost always found as a part of another compound. Therefore, to produce it, it has to be separated from the compound that contains it. One way to obtain it in-situ is through the electrolysis of water. Indeed, hydrogen repercussions on the overall carbon footprint of direct reduction greatly depend on the source of electrical energy. Only if the electrical energy comes from “green” sources (with

a carbon footprint lower than 130 gCO₂/kWh) are global emissions reduced with respect to the full natural gas case. This effect is disclosed in Table 4, where the three cases under investigation are further split into three subcases to analyze the sensitivity to different electrical energy sources.

Thanks to the different number of carbon-bearing species in the feed, when switching from Case 1 to Case 3, direct reduction process selective emissions show a drastic reduction, from 300 to 50 kgCO₂/metric ton DRI. Non-selective emissions, i.e., CO₂ emitted from process gas heaters, are reduced both because of less energy demand of the reactor and because tail gas sent to the heater is richer in hydrogen.

Figure 7



Results from Case 3: metallization, carbon and temperature maps.

Table 4

Carbon Footprint for Different Amounts of Hydrogen in the Feed and Considering Different Electrical Energy Sources									
	Case 1			Case 2			Case 3		
Electrical energy footprint [kgCO ₂ /kWh]	0.02	0.49	0.82	0.02	0.49	0.82	0.02	0.49	0.82
DRP selective emissions [kgCO ₂ /metric ton DRI]	300.77			126.63			49.82		
DRP non-selective emissions [kgCO ₂ /metric ton DRI]	194.51			160.14			150.83		
DRP electrical energy-related emissions [kgCO ₂ /metric ton DRI]	2.06	50.47	84.46	1.82	44.59	74.62	1.72	42.14	70.52
H ₂ production-related emissions [kgCO ₂ /metric ton DRI]	0	0	0	30.80	754.10	1,262.00	45.50	1,114.10	1,864.40
Total emissions [kgCO ₂ /metric ton DRI]	497.30	545.70	579.70	319.40	1,085.50	1,623.40	247.80	1,356.90	2,135.50

The direct reduction process already has a low electrical energy demand, and switching to higher hydrogen in the feed lowers it even more. On the other hand, electrical energy is required for hydrogen production and in cases 2 and 3 its source impacts very much on the carbon footprint. In the case of green or nuclear sources, the carbon footprint of Energiron ZR can be cut in half for the best case analyzed. On the contrary, if electrical energy is obtained from gas or coal, the carbon footprint of the DR process becomes twice or four times that of the natural gas-based one, respectively. It is therefore important that not only the steel-making industry but also the energy sector becomes carbon free to reduce global emissions.

Conclusions

A CFD study of an Energiron ZR shaft reactor was performed to compare results in terms of metallization, carbon content and discharge temperature as a consequence of different hydrogen amounts in the makeup gas.

One of the major effects of a higher hydrogen share is that a lower flowrate of bustle gas is needed. Since the overall endothermicity of the reactions is lower too, less energy must be supplied to the reactor and, as a consequence, the temperature of the bustle gas can be kept at a lower value.

The higher reactivity of H₂ provides a constant metallization value in the different cases, even if a slightly less uniform distribution of metallization is reached with higher hydrogen contents.

Furthermore, the reduction of natural gas injection in the cone of the reactor lowers the overall carbon content of the product, but this also means achieving a higher discharge temperature due to less endothermic reactions taking place in this part of the reactor.

The Energiron process is already known to be capable of handling high hydrogen content (virtually up to a full hydrogen feed) and to selectively separate CO₂ from the recycle gas, being able to reduce the direct emissions of carbon dioxide into the atmosphere.

An increased H₂ percentage in the feed gas, such as the one presented in this study, will prove beneficial in reducing GHG emissions even more, both from the process (with the possibility to avoid CO₂ removal with sufficiently high hydrogen contents as in Case 3) and from non-selective sources such as the fumes coming from the process gas heater. For this case in particular, the lower flowrate of bustle gas that has to be processed, together with its lower specific heat — and the lower temperatures — require a reduced flowrate of natural gas to the heater's burners, which ultimately leads to a reduced carbon footprint of the plant. In addition to the reduced environmental impact, the switch to hydrogen as presented in this

paper can lead to reducing energy consumption to 2.11 Gcal/metric ton.

Obviously, to have an impact on tackling CO₂ emissions, the hydrogen to be used for the reduction of iron ore has to be produced exploiting energy sources with a low environmental impact, such as electricity from green sources.

The CFD simulations shown in this paper allow for a fundamental understanding of the precise distribution of temperature, metallization and carbon content in the DRI inside the reactor by simply changing the composition in the boundary condition of the injected gas. Therefore, this has proved to be a valuable tool to evaluate the behavior of the Energiron reactor using different feed mixes in the process, and thus be fully prepared for hydrogen-based ironmaking.

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