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Simulation of Direct Reduction Processes to be included in a process chain multipurpose simulation toolkit

I. Matino, V. Colla, A. Vignali

Direct reduction is considered a suitable alternative process for the transition of steelmaking route towards C-lean processes. If direct reduction is performed with high percentage of hydrogen use in reducing gas, carbon dioxide emissions are expected to significantly decrease. However, investigations of the effects of integration of hydrogen-enriched direct reduction processes in existing steelmaking routes are required to provide steel companies with valuable guidelines for selecting the most economically, technologically and environmentally sustainable transitions steps. Therefore, within the EU-funded project entitled "Maximise H_2 Enrichment in Direct Reduction Shaft Furnaces" a first version of stationary flowsheet models of both Energiron-ZR and Midrex Direct Reduction processes were developed in Aspen Plus V14®. The models include shaft furnace and all auxiliary units and fit well with literature reference data. They will be used in a process chain multipurpose simulation toolkit to simulate the transition from standard integrated steelmaking route to a hydrogen-enriched direct reduction-based steelmaking route considering both production and gas and energy management aspects. In addition, these models will be the basis for dynamic models to investigate flexible operation of new integrated steelworks with hydrogen-enriched direct reduction.

KEYWORDS: DIRECT REDUCTION, STEELMAKING TRANSITION, PROCESS SIMULATION;

INTRODUCTION

The European steel sector is strongly affected by the European Green Deal. Since it accounts for about 20-25% of the industrial CO_2 emissions covered by the EU Emissions Trading System (ETS) [1], a significant reduction of its emissions is expected by 2030 and further reductions are needed to achieve the target of climate neutrality by 2050 [2]. To this aim, Direct Reduction (DR) of iron ore is considered one of the most promising technologies, especially if a high ratio of H_2 is used in the reducing gas [3]. Although different investigations are being carried out on this process [4-6], several aspects still need to be solved. One issue is related to the effect that the introduction of this new technology can have on configurations and management of existing integrated steelworks. As a gradual replacement of Blast Furnaces (BF) with combinations of DR shaft furnaces and Electric Arc Furnaces (EAF) are expected, significant changes will affect production, gas and energy management. To investigate how to optimally handle these aspect and the possible transition steps towards C-lean processes, within

Ismael Matino, Valentina Colla, Antonella Vignali
Scuola Superiore Sant'Anna, TeCIP, Pisa, Italy

the EU-funded project entitled "Maximise H_2 Enrichment in Direct Reduction Shaft Furnaces – MaxH_2DR" a process chain multipurpose simulation toolkit was developed [7]. A model library of standard and novel integrated steelworks technologies and units is included in the toolkit. Among them, two stationary flowsheet models are available to simulate DR processes, i.e. Midrex and Energiron Zero Reformer (ZR). Although in literature some models can be found [4; 8-10], they are generally too complex to be used in process chain simulations and optimizations, too specific or unavailable for inclusion in the toolkit, while the two models presented in the paper represent an acceptable compromise between accuracy and complexity, suitable to the general-purpose integrated steelmaking process chain analyses developed in the project.

MODELS FOR SIMULATING DIRECT REDUCTION PROCESSES

The two stationary models were developed in Aspen Plus® V14 according to literature data and information. The models allow considering both production, and gas and energy aspects and their computational complexity is low enough to simulate transition scenarios from a standard integrated steelworks to a fully H_2-DRI based steelmaking route, by thus enabling optimization studies related to production and energy streams distributions.

Midrex process model

Several literature works [4; 8; 10-13] and Midrex brochures/technical reports were analysed to acquire sufficient information and data to develop the model and assess its accuracy. The main operating parameters considered in the Midrex process model and the pellet main features are listed in Table 1.

Tab.1 - Midrex process model main operating parameters.

MIDREX MODEL MAIN PARAMETERS		
Parameter	**Unit of Measurement**	**Value**
Productivity	t_{HDRI}/h	321.5
Reformer temperature	°C	925
Shaft Furnace pressure	bar	1.5
Inlet reducing gas temperature	°C	>900
Pellet Fe content	wt%	67.1 (as Fe_2O_3)
Pellet SiO_2+Al_2O_3	wt%	3.8
Pellet CaO + MgO	wt%	0.1
Pellet P, S	wt%	traces

The main property method selected for the thermodynamic calculations is "SOLIDS" but in gas handling units "PENG-ROBINSON" is used, and the following list of components are considered in simulations: Fe, C, FeO, Fe_2O_3, Fe_3O_4, Fe_3C, SiO_2, Al_2O_3, CaO, MgO, P, S, CH_4, H_2, CO, CO_2, N_2, O_2, Ar and H_2O. The flowsheet of developed model is depicted in Figure 1.

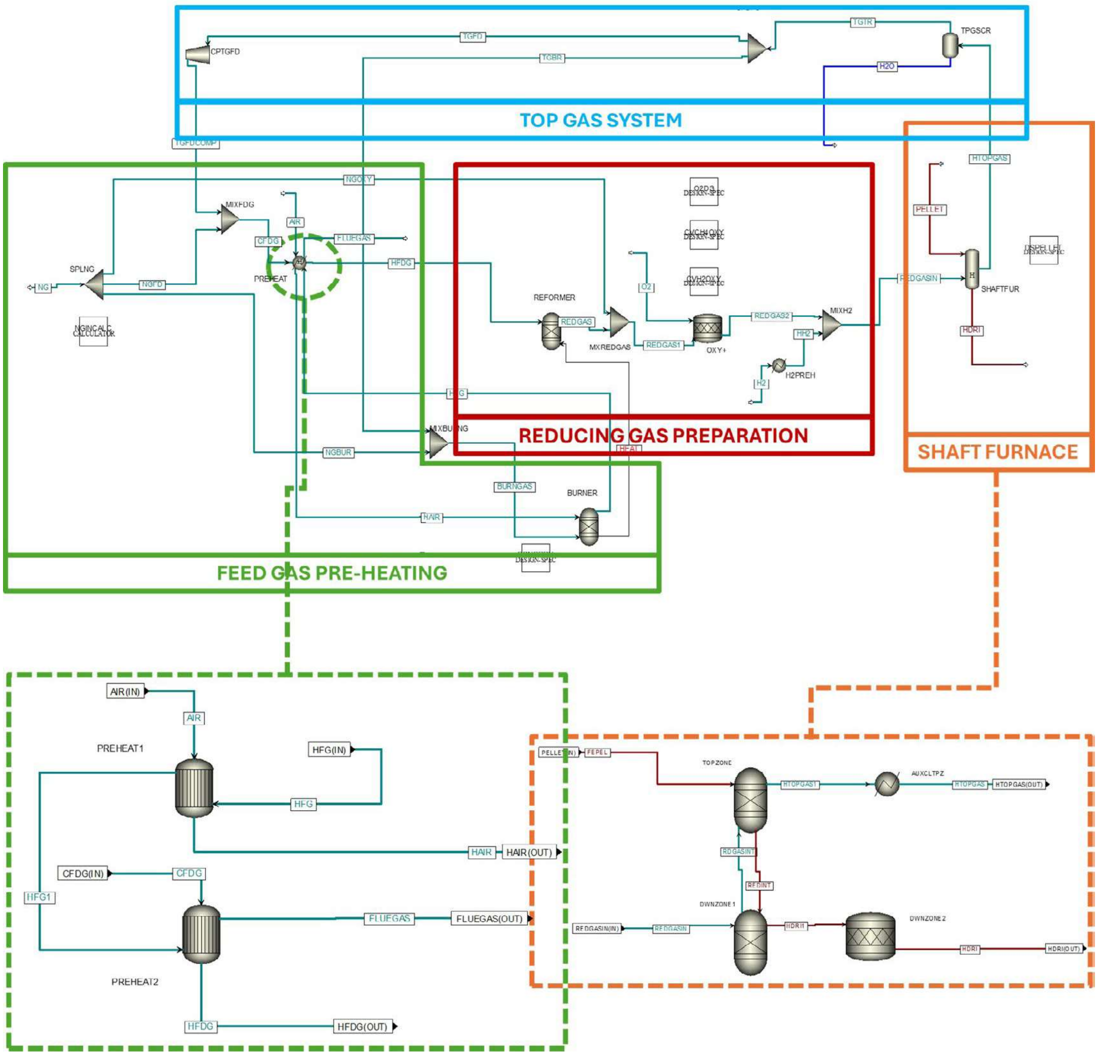

Fig.1 - Midrex process model flowsheet.

A combination of several units is used to simulate the main process sections: feed gas pre-heating, reducing gas preparation, shaft furnace, top gas system. In addition, different "Design-Spec" (DS) blocks and ad-hoc written "Calculator" blocks are included to controlling some process parameters and for considering specific aspects of the process. The feed gas pre-heating section starts with the inlet of Natural Gas (NG), here assumed as pure CH_4, that is split in three streams (i.e. for burner, to be sent in reformer and to be used in OXY+ unit). Then a burner is simulated through a RGIBBS reactor and a dedicated DS block, and fed with both NG and purged top gas. It provides heat for the reformer and for pre-heating combustion air and the gas to be sent to the reformer (i.e. a mix of NG and recycled top gas). The DS block provides adequate heat to the reformer to ensure a suitable operating reformer temperature. A "hierarchy" block (dashed green square in Figure 1) contains two HEATX units for heat exchange between hot streams (i.e. burner off-gases) and cold streams (i.e. combustion air and gas for reformer). The inlet gas to reformer is pre-heated at 500°C.

The section of reducing gas preparation includes the reformer, the OXY+ system and the possibility to add hydrogen. The reformer is modelled via a RGIBBS reactor and allows especially CO_2 reforming. OXY+ system is modelled as a combination of RSTOICH reactor and DS for controlling the O_2 feed and the partial oxidation of the gas to provide adequate H_2 and CO content in reducing gas, and to obtain the required reducing gas inlet temperature. Shaft furnace is represented as a HYERARCHY block with a combination of two zones (orange dashed square in Figure 1): the top zone (a further combination of RGIBBS reactor and a HEATER) allows especially reduction reactions, while the bottom zone (represented through a RGIBBS and a RSTOICH reactors) represents the finalization of reduction and the carburization. In this version of the model, the cooling section has been neglected and hot DRI (HDRI) is obtained. The last part of the model is related to Top Gas System that is currently very simplified. It includes a FLASH unit for removing especially water, a splitter for managing the recycling and purging of the gas and, finally, a compression stage of the recycled gas.

Energiron ZR process model

Literature analysis provided the basis also for the development of the Energiron ZR model [9; 11; 13-18]. An analysis of Energiron brochures/technical reports was also carried out to acquire further information and data. The main operating parameters considered in the Energiron ZR model are listed in Table 2; pellet features are the same as reported in Table 1. Main property methods and components considered in the model are the same as the Midrex model.

Tab.2 - Energiron ZR process model main operating parameters.

MIDREX MODEL MAIN PARAMETERS		
Parameter	**Unit of Measurement**	**Value**
Productivity	t_{HDRI}/h	321.5
Shaft Furnace pressure	bar	7
Inlet reducing gas temperature	°C	>1050

Figure 2 depicts the Energiron ZR model flowsheet. Also in this case, several units, DS and "CALCULATOR" blocks are combined to represent all the process sections, namely feed gas pre-heating, shaft furnace and top gas system. In the first section, NG and/or hydrogen (currently it is not used) are fed to the system, then their blend is split into a main part that is mixed with recycled top gas (forming the bustle gas) before being sent to the pre-heating, while the rest is fed to the burner to provide the heat for this preheating. Bustle gas preheating at about 900°C is simulated by using two HEATX units in series to exchange heat between burner combustion gas (hot stream) and two cold streams (i.e. bustle gas and combustion air). Before being preheated, the bustle gas passes through a humidifier, which is simplified as a combination of MIXER and DS blocks. It allows reaching the desired water content in the reducing gas (i.e. about 5-11 %vol. with higher values for lower H_2/CO ratio in bustle gas [18]). A final stage of partial oxidation of bustle gas is carried out using a RSTOIC unit and DS blocks to reach an operating temperature higher than 1050°C. Similarly to the Midrex model, the shaft furnace is simulated as a HIERARCHY block with two zones (dashed line square in Figure 2): the top zone is simulated via a RGIBBS reactor where mostly the reduction reactions take place, while the bottom zone is simulated via a RGIBBS and a RSTOIC reactors where, besides the finalization of reduction, mainly the partial oxidation and reforming of the bustle gas and the carburization reactions take place. Hot DRI is obtained from the shaft furnace unit model. Finally, the top gas system includes a cooler, which is simulated through a "HEATER" block to decrease the top gas temperature to 50°C and condense water (FLASH block), and to provide heat for the amine scrubber and the recycled top gas heating. After water removal, part of the top gas is sent to the burners of the pre-heating system, while the remaining part is compressed and sent to the amine scrubber for the CO_2 removal. The amine scrubber is currently simulated as characterized by a constant removal efficiency of 90% considering a liquid/gas ratio equal to 3 and computing related energy demand by using a relation obtained in SMARTER RFCS project [20]. After CO_2 removal, the treated top gas is heated and mixed with NG and H_2 to obtain the bustle gas to be preheated.

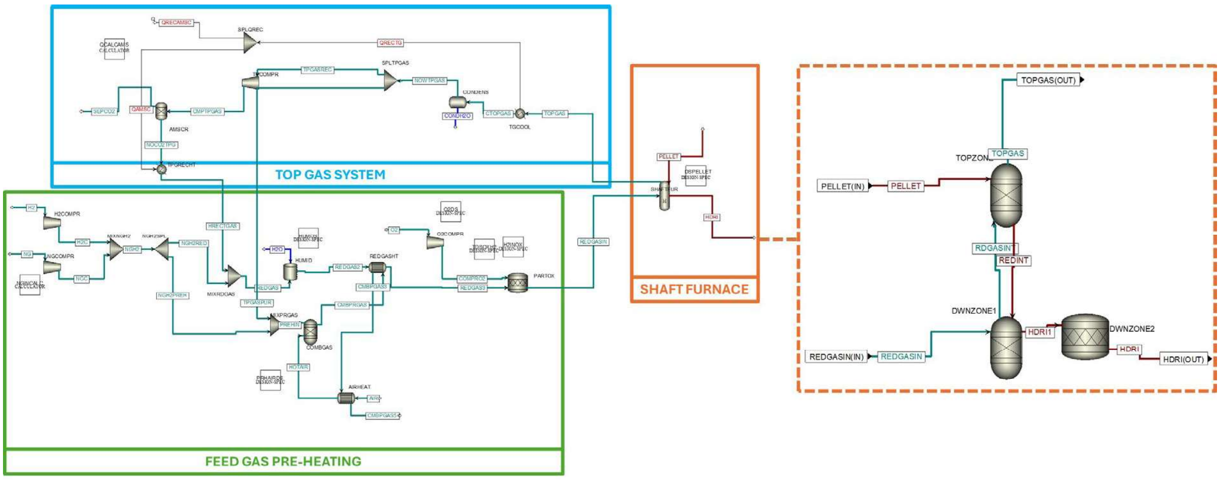

Fig.2 - Energiron ZR process model flowsheet.

NUMERICAL RESULTS

The results obtained with the models presented in the previous section are reported in Table 3 where they are compared to literature data [4; 8-18]. The results generally fit the reference values ranges, and the models can be considered accurate. However, further work will be done to improve them especially in case of higher differences with respects to reference data (e.g. O_2 consumption).

Tab.3 - Comparison of models results with reference data.

MIDREX AND ENERGIRON ZR MODELS RESULTS					
Variable	Unit of Measurement	Simulation	Reference	Simulation	Reference
		Midrex		Energiron ZR	
Iron Input Material	t/t_{DRI}	1.35	1.36-1.45	1.35	1.35-1.42
NG consumption	Nm^3/t_{DRI}	294.3	257-300	277.5	260-280
O_2 consumption	Nm^3/t_{DRI}	38.3	12-30	73.7	45-60
DRI metallic Fe	%wt	85	81-90	85	84.9-85.0
DRI Metallization	%	94	92-96	94	92-95
DRI C Content	%wt	2(50% as Fe_3C)	1-4	2(93% as Fe_3C)	1.5-4.5
HDRI Temperature	°C	657	650-730	605	600-700
Bustle Gas CO Content	%vol.	33.2	29.8-36.0	21.8	14.8
Bustle Gas H_2 Content	%vol.	52.6	49.7-55.0	48.1	47.9
Bustle Gas CH_4 Content	%vol.	6.0	5.9-9.0	17.4	19.5
Bustle Gas CO_2 Content	%vol.	2.1	2.2-2.5	2	1.7
Bustle Gas H_2O Content	%vol.	6.1	4.3-6.2	10.5	11.0
Bustle Gas Temperature	°C	904	887-980	1139	970-1100
Top Gas Temperature	°C	368	285-400	427	400-470

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CONCLUSIONS

DR processes are considered to investigate the transition of integrated steelmaking towards C-lean processes. In order to investigate the effects of their introduction in current integrated steelworks, Midrex and Energiron ZR models were developed to be used in a process chain multipurpose simulation toolkit to be exploited to evaluate transition effects on production and gas and energy management. The models were developed using literature data and their results fit with references variables values ranges. Further work is ongoing to improve their accuracy and robustness by acquiring information and operating data directly from technology providers and by using data that will be obtained during the other investigations carried out within the MaxH$_2$DR project. In addition, the presented stationary models will be the basis for the development of their dynamic versions.

ACKNOWLEDGMENTS

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