Process Integrated Modeling for the Classical Iron and Steelmaking Route and ULCOS Breakthrough Processes Life Cycle Inventory Analysis

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Life Cycle Assessment is nowadays a powerful method to compare the full range of environmental damages assignable to products, services or processes, in order to be able to assess them and to choose the least burdensome one. To perform the LCA, all the fluxes entering and exiting the chosen system must be assessed, which involves most of the time a difficult collection of data, called Inventory, which hardly verify mass and energy balances. From the precision of those data depends the accuracy of the LCA. If the system studied does not exist yet, as it is precisely the case for the ULCOS breakthrough processes, establishment of the inventory becomes uncertain.

To overcome this difficulty a novel method has been developed, in the framework of ULCOS SP9 WP2, which consists in replacing the traditional inventory data collection by a rigorous process modelling step which provides all the data required for the Inventory. Such a methodological coupling of process modelling and LCA permits rigorous assessment of existing processes and future ULCOS processes as well.

Introduction

It is now commonly recognised that CO_2 emissions are the major factor of the global warming effect. In order to meet Kyoto requirements, the European Steel Industry has decided to integrate environmental considerations into the traditional product design process, for powerful eco-efficiency, and has created the challenging ULCOS (Ultra Low CO_2 Steelmaking) consortium that has taken up the mission to develop breakthrough steelmaking process with the potential to reduce CO_2 emissions by a factor of 2 [1].

In order to assess the current steelmaking route and to unable the design and the development of new ones with better environmental performances, Life Cycle Assessment (LCA) method was chosen.

Life Cycle Assessment method was retained in ULCOS as the most holistic approach of assessing environmental impact and selecting new technologies. Previous to the impact assessment, it is essential to carry out the Life Cycle Inventory (LCI) of the process, which is the core part of LCA methodology. According to the current LCA standards [2], the quality of the data used for carrying out this inventory is one of the most important limiting factors. The LCI analysis involves data collection, calculation and procedures to quantify the relevant inputs and outputs of the product system. The data collection should correspond to some conditions: precision, completeness, representativeness, consistency and reproducibility [2]. It is obvious that such conditions are not easy to respect. The environmental performance of complex steelmaking processes such as iron ore sintering are strongly dependent on operational conditions and can change significantly when different types of fuels and recycled wastes are used in the process.

Moreover, data used for inventory calculation should also respect exigencies such are the age, the geographical and technological coverage. In many cases, the environmental data related to the steelmaking industry cannot be used due to the lack of measurement of certain pollutants or because the information is much too summarized. It is clear that LCA practitioners are confronted with serious difficulties in respecting these conditions when the LCI is based only on data coming from literature and/or industrial practice. Also, it is generally recognized that the classical approach of assessing LCI takes time, and usually it cannot guarantee the mass and energy balances of flow rates which are considered in the system boundaries.

It is therefore crucial to improve the way of assessing the LCI of the steelmaking industry in order to guarantee the quality of the data and to predict the change of the environmental performances with respect to the operational conditions.

Methodology

In the frame of the ULCOS project, the objective of our work was to develop a new methodology which combines the process integrated model approach with LCA in order to improve the way of assessing the LCI for steel production [3], see Figure 1.

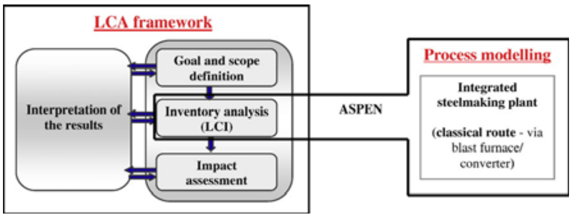

Figure 1. Methodological coupling between LCA and process modelling

Based on physicochemical considerations, thermodynamics laws and mathematical equations, Aspen Plus software have been used in order to develop modules for each steelmaking processes as presented in Figure 2 (coke plant, sinter plant, blast furnace, basic oxygen furnace, continuous casting and hot rolling). Aspen Plus (Advanced System for Process Engineering) is a process engineering software package that is used to simulate processes based on thermodynamic models, properties of materials and several built-in unit operation models.

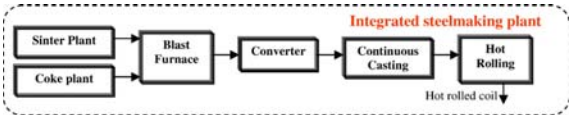

Figure 2. Classical integrated steelmaking plant

The modules developed calculate the mass and heat balances, emissions, and the chemical compositions of products and by-products simultaneously.
The challenge in our work was to develop models which are a trade-off between complexity and accuracy. Indeed, these models are quite simplified compared to sophisticated models already existing for each steelmaking processes, but however complex enough to allow us the calculation of the amount of various pollutants. Furthermore, the amounts and the composition of products and by-products such as the steelwork gases are also calculated. This last information is very important because the steelwork gases (coke oven, blast furnace and converter gases) are used as fuels by all of the steelmaking processes described in Figure 2. Consequently, the contribution of these gases to the total environmental burden of the system can be easily estimated.
Details concerning the different modules have already been presented elsewhere, see [4, 5, 6].
Each module was validated against industrial data coming from Arcelormittal plants, as well as against data from a Voestalpine blast furnace. Calculations with those industrial data showed very good results, mostly within 5 % of the plant measured values.
Finally all the different modules were connected together by each primary product and any possible by-product interactions, in order to build a macro steelmill simulator, and the inventory of the steelmaking process has been easily carried out.

Validation of the methodology

Two Aspen Plus simulations have been carried out [6] in order to check the results of the approach developed. Data used for those calculations respectively comes from:

- industrial data supplied by a European integrated steelmaking plant,
- "benchmark" data supplied by the ULCOS project. In the frame of the ULCOS project, the "benchmark" data defined an integrated steelmaking plant characterised by the best available technologies.

In addition, a reference LCI database developed by the International Iron and Steel Institute (IISI) was used to allow further comparison. This reference LCI has been developed on the basis of fourteen worldwide steel plants [7]. For all three cases, LCI are reported at the same functional unit, which is the production of one ton of Hot Rolled Coils. LCI was performed with GaBi software. Comparison of CO_2 emissions between the three simulations is outlined in figure 3.

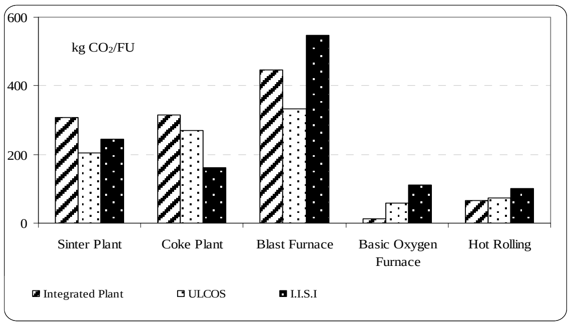

Figure 3. Inventory of CO_2 emissions for each process included in the analysed system

According to this figure, the total CO_2 emission released by the defined processes is: 1147 kg/FU (European integrated plant); 937 kg/FU (ULCOS benchmark) and 1165 kg/FU (IISI reference case). These CO_2 emissions are calculated for each process without taking into consideration the consumption of electricity. CO_2 variance between the analysed cases is basically linked to the differences in amounts of raw and intermediate materials (coke, sinter, hot metal...) used in the process. Moreover, the use of various types of fuels for heat supply: blast furnace, coke oven, converter and natural gases, can also contribute to the variation of emission due to the chemical composition and the heat capacity of these gases.

Electricity required by the system is supplied by internal production using steelworks gases, namely blast furnace gas, coke oven gas and converter gas, which are considered as by-products of coke, hot metal and steel plants. Not the entire amount of steelworks gases produced in the system is consumed only for electricity generation. Actually, prior to electricity production, some of the gases are used in the system as heat supply for coke oven heating, hot rolling stoves, and blast stoves as indicated in Figure 4.

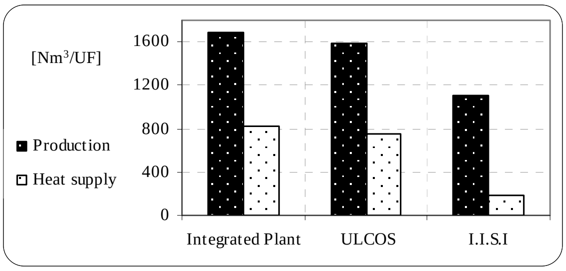

Figure 4. Steelworks gases production and internal consumption as heat supply

The difference between the production of these gases and their consumption as heat supply was called "excess of steelworks gases". This excess is used mainly for internal electricity production but also as an energy supply for auxiliary facilities such as raw materials preparation, lime production and steam production. For the current LCA study these facilities are not considered in the system boundaries.

The production of electricity using steelworks gases was also simulated with a simplified Aspen Plus module developed for an internal power station. The CO_2 emissions calculated with this module for the production of electricity required by the system are given in table 1.

Table 1. CO_2 emissions involved in the integrated steelmaking plant

CO_2 emission [kg/FU]	Integrated Plant	ULCOS	IISI
Steelmaking Processes	1147	937	1165
Electricity production	440	510	499
System total emissions	**1587**	**1447**	**1664**
Auxiliary facilities	362	293	344
Total	**1949**	**1740**	**2007**

Table 1 also sums the amount of CO_2 released by the production of one ton of hot rolled coil as defined by the system boundaries. CO_2 emissions for the ULCOS benchmark are significantly lower than the other scenarios. This can be explained by the fact that ULCOS scenario is based on the consumption of a large amount of pellets in the blast furnace. The environmental burden of pellet production is lower than the burden of sinter production. In addition, in the ULCOS scenario, the coal injection in the blast furnace reaches the maximum rate and consequently the consumption of coke is reduced. Indeed, the decrease of coke demand leads to lower environmental burden for the system. The CO_2 emissions calculated by the model for the European steelmaking plant were successfully compared to the average value of fourteen plants derived from the IISI inventory. This result emphasizes the accuracy of the model and fortifies the reliability of the proposed approach.

According to [3] industrial experience shows that there is no excess of energy when all the auxiliary facilities (raw materials preparation, lime production, steam production) are part of integrated plant. If the system boundaries are extended towards auxiliary facilities, the environmental burden involved in the total consumption of steelworks gases in the frame of the system should be integrated into the LCA study (see table 1 for CO_2 emissions). Thanks to the current approach, it has been shown that by using the best available techniques and optimizing the use of resources, the environmental burden can be notably reduced. To exemplify, the CO_2 emissions can be reduced by 200 kg of CO_2/FU for the ULCOS benchmark case.

Predictive LCI

The integrated steelmaking plant constitutes the actual reference for the classic steelmaking route. The modules developed to simulate the different processes of this integrated steelmaking plant were all validated on the basis of industrial data and proved their ability to generate accurate life cycle inventories. Once this method has proved valid it can be extended to other systems, which can be modelled with Aspen Plus. In this regard, models for the Direct Reduction route, e.g. MIDREX process, are currently developed, in order to draw a comparison with the blast furnace route, in terms of CO_2 emissions.

But the main feature of this methodological coupling between flowsheeting and Life Cycle Analysis, lays in the ability to study processes that do not exist yet. Indeed for such processes, drawing the life cycle inventory with the classical data collection is not possible. The only way to produce an accurate life cycle inventory with such processes is to go through a physico-chemical modellisation step that ensure mass and energy balance, and verify fundamentals laws of physics and chemistry.

In the framework of ULCOS, several breakthrough processes were imagined and designed to produce iron with limited CO_2 emissions. Those processes are currently being modelled via simplified physico-chemical models and integrated into complete Aspen Plus flowsheets to generate LCI of those new routes.

Once done, a relevant comparison between the classical reference route and the breakthrough routes proposed in the framework of ULCOS will be possible. Such a comparison will help to assess the different possibilities that are offered and to choose the less burdensome for the environment.

In addition the process unit models developed in this framework allows to test easily different configurations of the flowsheet (distribution of gases, production of steam, electricity ...) and in this way, they are helpful tools for optimal design of the whole process.

Currently, our study is focused on Aspen Plus modelling of the new ULCOS steelmaking routes, starting with the new DRI process, ULCORED [8]. The flowsheets proposed in the framework of ULCOS Sub Project 12 were selected as the basis for our calculations.

Model assumptions

Main features of the new process proposed in the framework of ULCOS (Sub Project 12) may be found in ULCOS reports (see Figure 5 for schematic flow-sheet).

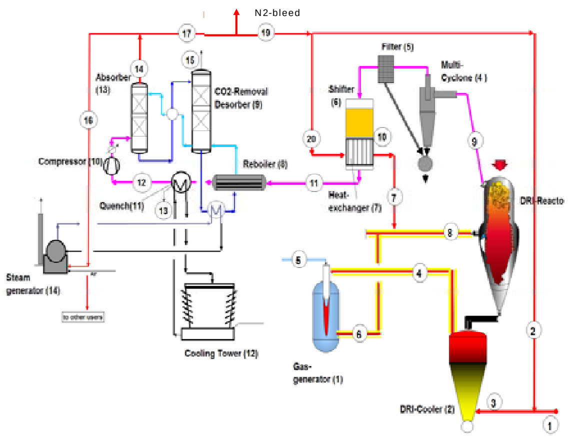

Figure 5. ULCOS SP12 flowsheet for ULCORED process

Basically natural gas is mixed with a fixed amount of clean recycled gas before going through a DRI cooler that acts like a preheater for the gas mixture. The gas temperature at the exit of the cooler is calculated from the DRI inlet and outlet temperatures in the cooler, and the carburization degree of the DRI (carburization is assumed to take place into the cooler). The preheated mixture then goes through the syngas generator (POX), where the amount of added oxygen depends on the operating temperature. The composition of the syngas at the POX outlet is calculated assuming a thermodynamic equilibrium (Gibbs approach). The syngas is then mixed with clean preheated recycled gas. The amount of recycled gas used at this step depends on the amount previously mixed with natural gas. The gas then enters the shaft where it reduces the pellets. The composition of the gas at the shaft exit is calculated with the assumption of an equilibrium (water gas shift reaction) at 700°C. The remaining CO is then shifted into CO_2 (exothermic reaction). Heat produced by the 2-stage shifter is used to preheat recycled gas and produce steam. The gas is then cooled to 40°C and the water condensed is removed from the system, before the gas enters the CO_2 removal system (PSA+cryogenics). CO_2 is removed from the gas which is partially purged before going into the recycling loop. The amount of purged gas has to be high enough to ensure acceptable nitrogen content into the recycling loop.

Input data of the model are summarized in Table 2.

Table 2. Input data of the ULCORED model

INPUT DATA		
Pellets	Composition	ULCOS SP9
	Humidity	2%
	Nitrogen introduced	0,8 $Nm^3/t_{pellets}$
DRI	Weight	1 ton
	Metallization	93%
	Carburization	2,75%
	Discharge Temp.	45°C
	Temp. at shaft exit	900°C (variable)
	Cooler heat loss	50 MJ/t_{DRI}
Natural Gas	Composition	ULCOS SP9
Oxygen	Purity	99,8%
POX	Inlet gas flow	Variable
	Operating T	1200-1400°C
	Heat loss	50 MJ/t_{DRI}
Shaft	Bustle gas T	910°C
	Top gas T	400°C
	Shaft heat losses	100 MJ/t_{DRI}
Shifter HT	CO at exit	2,8%
Shifter LT	Input T	220°C
	CO converted at exit	99,97 %
PSA+CRYO	Efficiency	3% CO_2 at exit
	CO recovery	97,5%
	N_2 recovery	99%
	H_2 recovery	100%
Purge*	Flow	30 Nm^3

* purge flow ensures a volume fraction of nitrogen less than 10% in bustle gas.

From those data, the simulating tool calculates the output data summarized in Table 3.

Table 3. Outputs of the ULCORED model

OUTPUT DATA	
Weights	Pellets
Flows	Oxygen Natural gas Vapour produced Cooling water Water removed from the system Recycling loop flow required to ensure energy balance
Gas compositions	Everywhere in the system Captured gas Purged gas
Temperatures	Preheated recycled gas POX inlet

POX model

A special attention was given to the partial oxidation reactor (POX), which is intended for preparing syngas from natural gas. In a first approximation, the easiest way to model the POX is to suppose a thermodynamic equilibrium at given temperature and pressure, and to calculate the composition that minimises the Gibbs energy. Nevertheless such an approach may be inadequate if the reaction kinetics prevent from reaching thermodynamic equilibrium. As Aspen Plus does not feature reaction kinetics (unless kinetics are known, which is not the case), it was decided to make proper, rigorous kinetic calculations using the CHEMKIN4 software (in collaboration with DCPR, Nancy-Université).

Calculations were carried out assuming a plug flow reactor operated in the conditions stated by SP12 (Table 4).

Table 4. Operating conditions of the POX

Inlet gas composition	
H_2	61.0 %
CO	0.0 %
CO_2	0.0 %
H_2O	1.5 %
CH_4	35.5 %
N_2	2.6 %
Inlet gas flow rate	700 Nm^3
Inlet gas T	520 °C
Oxygen flow rate	170.9 Nm^3
Outlet gas T	1200 °C
POX pressure	6 bars

The evolution of the composition of the outlet gas as a function of residence time in the POX (Figures 7 and 8) reveals that, under such conditions, the time required to reach equilibrium (200 s) largely exceeds the residence time in the reactor (envisaged about 4 s).

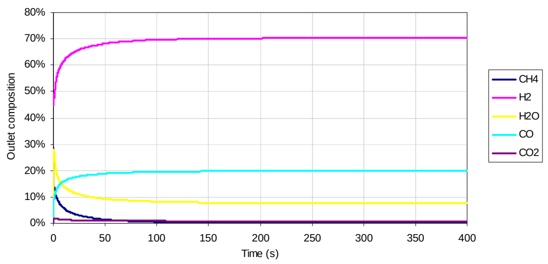

Figure 7. Evolution of the outlet gas composition at 1200°C as a function of residence time

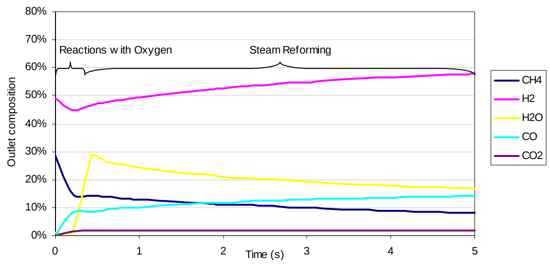

Figure 8. Detail of the composition for the first five seconds

Indeed partial oxidation competes with the reactions of total combustion and of hydrogen oxidation. These reactions are very fast and only after oxygen has totally reacted can the residual CH_4 (about half of the initial amount) slowly react by steam reforming to finally reach thermodynamic equilibrium. Those conditions thus apparently would fail to produce the desired syngas by the system. Other calculations showed that pressure little influences the outlet composition. Conversely, temperature is a critical parameter. If the temperature in the POX is lowered (and oxygen flow rate adjusted) the situation is even worse (oxygen reacts preferentially with hydrogen), but if the temperature is increased to 1400°C (and oxygen flow rate adjusted as well) the outlet composition may reach acceptable state in reasonable time. At this temperature a composition close to equilibrium is reached within 2 to 3 seconds, which matches the expected residence time in the POX. Nevertheless, before reaching equilibrium, the gas goes through a short period during which the formation of soot is very likely (CHEMKIN4 cannot evaluate this phenomenon).

First results

Results of the simulations agree well with calculations made using the IRMA software (CORUS, SP12). It was decided to run calculations with a POX at 1400°C. This temperature should ensure a good behaviour of the POX, as discussed in the previous paragraph. Different distributions of the recycled gas into the system were tested and showed that a diminution of the POX inlet gas flow rate may lead to a reduction of oxygen and natural gas consumptions. On the other hand with an increase in the POX inlet gas flowrate to 807 Nm^3, the system could operate without any heat exchanger for the recycle gas, as shown in Figure 9.

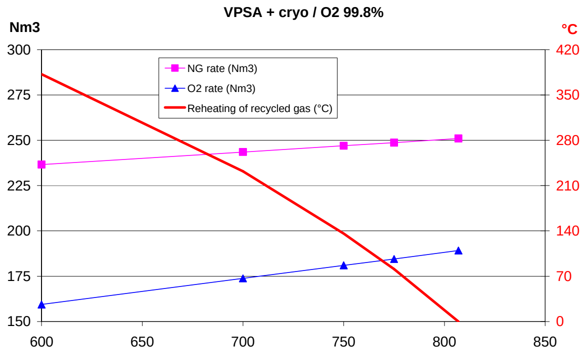

Figure 9. Effects of POX inlet gas flowrate on Natural Gas and Oxygen Consumption and recycled gas preheating

Those first results clearly showed that this Aspen Plus tool can be used very easily to generate accurate data for the Life Cycle Inventory Analysis, but also to work on the flowsheet optimization in a broader framework.

The model developed is now ready to be coupled with GABI4™ LCA software.

Conclusion

A novel methodology, coupling flowsheeting and LCA, was developed in the framework of this study. Simplified physical-chemical models of unit processes is an efficient way to establish accurate Life Cycle Inventory for existing processes without going through the classical data collection step, and also gives predictive LCI for processes that do not exist yet.

This methodology enables us to control the mass and energy balances of the calculated inventory, something that is nearly impossible to assure when the LCI is carried out using only average data from literature or experimental works. Secondly, calculating emissions based on physicochemical and mathematical considerations gives a strong credibility to the inventory.

This methodology was first tested applied to an existing integrated steelmaking plant and showed very good results.

It was then extended to the breakthrough Direct Reduction process ULCORED for which modelling is the only way to get LCI data. The model developed showed very good ability to test and evaluate different operating conditions of the process and the best scenario can be identified in minimal time.

Acknowledgements

The present work is part of the ULCOS program, which operates with direct financing from its 48 partners, especially of its core members (ArcelorMittal, Corus, TKS, Riva, Voestalpine, LKAB, Saarstahl, Dillinger Hütte, SSAB, Ruukki and Statoil), and has received grants from the European Commission under the 6th Framework RTD program and the RFCS program[1].

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[1] Priority 3 of the 6th Framework Programme in the area of "Very low CO_2 Steel Processes", in co-ordination with the 2003 and 2004 calls of the Research Fund for Coal and Steel