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Techno-economic assessment of the INITIATE process

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Abstract

The iron and steel industry along with the fertilizer one are the most energy and carbon intensive representing roughly the 30% of all industrial CO_2 emissions. The aim of this work is to assess the techno-economic analysis of the INITIATE process for reducing the carbon footprint of integrated steel mills and simultaneously producing valuable chemical products such as ammonia and/or urea. The core of the INITIATE process is given by the Sorption Enhanced Water Gas Shift (SEWGS) technology that allows the industrial symbiosis between the steel and the urea industries, by treating the residual steel gases (i.e. BOFG and BFG) and producing a CO_2 rich stream, suitable for storage or utilization and a H_2/N_2 stream that can be used for ammonia synthesis but also to be recycled back to the steel plant to cover part of its heat demand. Two different sizes of the INITIATE process, in terms of urea production have been investigated and compared to base and reference cases. The techno-economic analysis shows the advantages given by the industrial symbiosis by an environmental and economic point of view. The small-scale INITIATE plant shows a negative SPECCA for a low-carbon electricity scenario and a negative CCA for a wide range of the cases investigated in the sensitivity analysis. The large-scale INITIATE plant presents a lower SPECCA with respect to the reference plants when the electricity carbon footprint is lower than 250 kg_{CO2}/MWh, while by an economic point of view, the large-scale INITIATE plant is advantageous with respect to the corresponding reference plants especially in the case of high natural gas prices. On the other hand, the large-scale INITIATE plants can achieve a reduction of the carbon footprint equal to 87%.

Keywords: Industrial symbiosis; steel; ammonia; urea; SEWGS; CCUS; GHG; CO_2 mitigation

1. Introduction

The currently deteriorating climate crisis imposes the adoption of urgent actions to mitigate its economic and social consequences, starting from a drastic and rapid reduction of anthropogenic greenhouse gas (GHG) emissions. It is thereby crucial to reduce industrial GHG emissions, which contribute significantly to the total anthropogenic carbon footprint. The steel and the fertilizer sectors are, specifically, two of the most energy and carbon intensive representing roughly the 30% of all industrial CO_2 emissions [1]. The INITIATE project aims to demonstrate a novel and symbiotic CO_2 utilization process that exploits the residual gases from the steel industry (i.e. BOFG and BFG) for urea production. The coupling of these two manufacturing processes can be achieved by converting the residual steel gases into NH_3 and CO_2, feedstocks for the urea synthesis. The INITIATE concept has thus the potentiality of reducing the

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emissions related to the steel and urea production, but also of making Europe more self-sufficient in the fertilizer production contributing at the same time in the development of a value chain related to carbon capture and utilization.

Nomenclature

BF	Blast Furnace
BFG	Blast Furnace Gas
BOF	Basic Oxygen Furnace
BOFG	Basic Oxygen Furnace Gas
CCA	Cost of CO_2 avoided [€/t_{CO2}]
CCS	Carbon Capture and Storage
CI	Carbon Intensity
COG	Coke Oven Gas
GHG	Greenhouse Gases
GT	Gas Turbine
HRC	Hot Rolled Coil
HRSC	Heat Recovery Steam Cycle
HRSG	Heat Recovery Steam Generator
LHV	Lower Heating Value [MJ/kg]
MDEA	Methyldiethanolamine
MEA	Monoethanolamine
NG	Natural Gas
PEC	Primary Energy Consumption [GJ/$t_{product}$]
SEWGS	Sorption Enhanced Water Gas Shift
SPECCA	Specific Primary Energy Consumption for CO_2 Avoided
TEC	Total Equipment Cost [€]
TPC	Total Plant Cost [€]
WGS	Water Gas Shift

1.1. Carbon capture and storage in steel plant

In order to reduce the carbon footprint of the steel sector, different solutions have been studied or are under investigation. Approximately 50% of the steel plants' CO_2 emissions are concentrated in the power generation off-gases. The rest is mainly associated to distributed process heat generation, resulting in various emission points. Post-combustion carbon capture technologies, such as monoethanolamine (MEA) solvent scrubbing based process, can be applied to power generation section only, or also to the other abovementioned emission sources even if the second option is very challenging since many different small capture section would be required [2]. Another option to reduce the carbon footprint of the steel plants is the application of precombustion carbon capture technologies removing the carbon content of the steelworks arising gases which can be used as clean fuel for power production and to cover the thermal requirements of the steel plant [2]. Among all the precombustion technologies, the Sorption Enhanced Water Gas Shift process represents a promising alternative for the decarbonisation of the steel industry [2], [3], [4], [5]. The SEWGS reactor simultaneously produces two streams, one rich in CO_2, suitable for storage or utilization, and another rich in H_2/N_2 that can be used as clean fuel or as feedstock for the synthesis of chemicals.

1.2. Objective of the work

The aim of this work is to assess the techno-economic analysis of the INITIATE process. Different plant configurations and sizes are investigated and compared to the base cases (conventional production of steel and urea) and the reference cases (steel plant with pre-combustion CO_2 capture using MDEA scrubbing and ammonia plant with post-combustion CO_2 capture using MEA scrubbing). In the following sections the different investigated configurations are described more in detail.

2. Investigated plant configurations

2.1. Base cases

As briefly introduced before, the base cases represent state-of-the-art commercially available plants. The size selected for the base steel plant is 3.16 Mt_{HRC}/y while for the ammonia/urea base plants two different sizes are considered as reported in Table 1 (last column refers to capture technologies adopted in the reference cases and described in section 2.2).

Table 1: Base cases

Plant	Product	Size	Technology	Application	Reference case CO_2 capture
Steel plant	Hot rolled coil	3.16 Mt/y	BF-BOF		MDEA pre-combustion
Ammonia plant	Ammonia	128 t/d	NG steam reforming	Coupled with urea plant	MEA post-combustion
	Ammonia	848 t/d	NG steam reforming	Coupled with urea plant	MEA post-combustion
Urea plant	Liquid urea	224 t/d	Conventional	AdBlue	Not applicable
	Liquid urea	1500 t/d	CO_2 stripping	Liquid fertilizer	Not applicable

2.2. Reference cases

Reference cases are defined as state-of-the-art plants with CO_2 capture commercially available technologies (see last column of Table 1). The size of the plants is the same as the base cases. In the case of the steel plant, a WGS+MDEA section is added to decarbonize the BFG+BOFG mixture before being sent to the combined cycle power plant. In the ammonia reference plants, a MEA post combustion section is added to decarbonize the flue gases from the primary reformer. On the other hand, in the case of urea plants no additional CO_2 capture sections are considered since in urea plants direct CO_2 emission sources are absent.

2.3. INITIATE case

Two different configurations of the INITIATE process are developed depending on the amount of steel gases processed by the SEWGS and later converted into ammonia/urea.

2.3.1. Small-scale INITIATE plant

In the small-scale INITIATE plant configuration, all BOFG available in the steel plant is treated in the WGS+SEWGS section. Consequently, the urea produced in this case is limited to the same amount of the small-scale base and reference cases. As can be inferred, the BOFG is no more available for power production or to cover part of the internal uses. In order to substitute the BOFG originally used for heating purposes, part of the BFG normally sent to the power block is mixed with natural gas. This becomes necessary to meet the requirements in terms of adiabatic flame temperature as the BFG lower heating value is much less than for BOFG. Therefore, the electricity produced internally is reduced because no BOFG is used in the power plant but also because less BFG is used to produce electricity. Consequently, it becomes necessary to import some electricity from the grid. On the other hand, the steam necessary for the water gas shift reactors, the SEWGS and the urea plant is produced by exploiting the heat available in the plant and using the purge gas from the ammonia loop as fuel.

2.3.2. Large-scale INITIATE plant

In the large-scale INITIATE plant configuration, all the available BFG and BOFG are sent to WGS+SEWGS section in order to be decarbonized. This means that no more BOFG and BFG are available for electricity production and to cover the heat requirements of the steel plant. Therefore, all the electricity necessary to run the steel plant is imported from the grid, while NG is imported to substitute the BFG and BOFG in the steel plant internal uses. In this plant configuration becomes necessary the adoption of a membrane to respect the ratio between hydrogen and nitrogen set by the ammonia process. Indeed, if in the case of the small-scale plant this equipment is not necessary, being the ratio between CO (that is converted into H_2 in the WGS stages) and N_2 in BOFG not so far from stoichiometric conditions, in the case of the large-scale plant the ratio between CO and N_2 in the BFG+BOFG mixture is so low that the excess of nitrogen has to be removed. The mass flow rate of the H_2/N_2 mixture sent to the ammonia loop is the one suitable to produce 848 t_{NH3}/d equivalent to 1500 t_{urea}/d. Part of the H_2/N_2 mixture that is not used to produce ammonia is burnt to produce IP steam while the rest is used to cover some of the heat demands of the steel plant. In addition, the rest of the steam necessary for the water gas shift reactors, the SEWGS and the urea plant is produced by exploiting the heat available in the plant and using the purge gas from the ammonia loop as fuel.

3. Methodology

3.1. Thermodynamic assessment

The methodology and the assumptions made to perform the thermodynamic assessment are reported in this section.

3.1.1. Steel plants

The steel plant considered in this study is representative of a plant located in Europe with an annual production of 3.16 Mt of hot rolled coil. The distribution and the composition of the gases in the steel plant is reported in Table 2. The power requirement of the steel plant, equal to 410 kWh/t_{HRC} is fully satisfied by the electricity produced in a combined cycle composed by two gas turbines and a 3 pressure levels heat recovery steam cycle where BFG and BOFG are used as fuel. The combined cycle has been simulated in Aspen Plus V11 selecting PENG-ROB equation of state.

In the case of the reference steel plant the decarbonization of the BFG+BOFG mixture going to the power plant has been simulated in Aspen Plus V11 using the ELECNRTL method and considering a MDEA carbon capture section. The CO_2 captured is then compressed to 110 bar.

Table 2: Gas streams distribution and composition in the steel plant

Stream	Mass flow [kg/s]	LHV [MJ/kg]	Molar composition [%mol]								
			H_2	N_2	O_2	CO	CO_2	Ar	H_2O	CH_4	HC ($C_{2.5}H_5$)
BFG internal use	157.49	2.28	2.4	53.5	0.0	22.7	21.4	0.0	0.0	0.0	0.0
BFG power plant	125.10	2.28	2.4	53.5	0.0	22.7	21.4	0.0	0.0	0.0	0.0
BOFG internal use	8.09	5.50	3.3	18.8	0.0	56.4	20.8	0.6	0.0	0.0	0.0
BOFG power plant	4.35	5.50	3.3	18.8	0.0	56.4	20.8	0.6	0.0	0.0	0.0
COG	7.65	39.32	59.5	5.8	0.2	3.8	1.0	0.0	4.0	23.0	2.7

3.1.2. Ammonia and urea plants

The simulation of the ammonia and urea plants has been carried out in Aspen Plus V11. The ammonia plant was simulated with the RKS-BM method, except for the clean-up section where the ELECNRTL method was used. The main operational condition and assumptions made for the simulation of the ammonia plant are reported in Table 3.

It is assumed that for the small-scale ammonia plant all the equipment are electrically driven meaning that all the electric power necessary for the plant is imported from the grid. On the other hand, in the large-scale ammonia plant the main equipment (i.e. compressors) are driven by steam turbines, exploiting the steam generated in the plant.

In the case of the reference ammonia plants, the decarbonization of the flue gas from primary reformer is performed in a MEA post combustion carbon capture plant that has been simulated with the ENRTL-RK method. The urea plants have been simulated using the SR-POLAR method. The steam input of the small-scale urea plant, being based on a conventional total recycled process, is assumed to be double the amount needed for the large-scale one.

Table 3: Ammonia and urea plants electric and steam input

Parameter	Unit	Small-scale	Large-scale	Parameter	Unit	Small-scale	Large-scale
Ammonia plant power consumption	MWh/t_{NH3}	1.4	0.7	Urea plant power consumption	kWh/t_{urea}	20	20
Ammonia plant power imported from the grid	GJ/t_{NH3}	11.2	0.3 [6]	Urea plant steam input	GJ/t_{urea}	4.4	2.2 [6]
Ammonia plant steam input	GJ/t_{NH3}	-7.7	-3.9 [6]				

3.1.3. INITIATE process

The INITIATE process is simulated in Aspen Plus V11.1 with RKS-BM method. The steel gases, sent to the INITIATE plant, are compressed from 1 bar to 17 bar. Two WGS reactors are adopted, feeding the first reactor with only 50% of the total gas mixture. The H_2O/CO ratio at the inlet of the first reactor is equal to 3 while at the inlet of the second one it is equal to 2. The overall H_2O/CO ratio is equal to 1.56. The WGS are simulated in Aspen Plus as adiabatic reactors adopting REquil model with an inlet temperature of 320°C. The SEWGS operation was optimized using a proprietary cycle model developed by TNO [7], [8], [9]. This model simulates a certain cycle design taking the relevant kinetics and adsorption equilibria into account. The simulations result in a full characterization of the cycle, steam consumption rates, number and sizes of columns and the compositions of the CO_2 and H_2 rich product streams. These results are then incorporated into Aspen plus by adopting a calculator and some other native equipment. The methanator reactor, with an inlet temperature of 250°C is simulated using a RGibbs reactor. The H_2/N_2 mixture that is sent to the ammonia loop is compressed till 312 bar while the recycle gas compressor inside the ammonia loop increases the pressure to 325 bar.

3.2. Economic assessment

In the following sections, the assumptions and the methodology adopted for the assessment of the economic model are described. For each analyzed case, the CAPEX and OPEX are computed. General assumptions, valid for all the plants are resumed in Table 4. Parameters which are not shown are assumed from previous publications [2], [5], [10].

Table 4: General economic assumptions

	Unit	Value
Natural gas price	€/GJ (LHV)	20
Electricity price	€/MWh	150
CO_2 transport and storage	$€/t_{CO2}$	10
Carbon tax	$€/t_{CO2}$	0

3.2.1. Steel plants

The total steel plant cost without the power generation section is adapted from [2] on the basis of the steel annually produced while the cost of the power plant and the cost of MDEA carbon capture section were computed according to the methodology described in [10].

3.2.2. Ammonia and urea plants

The total plant cost of the base ammonia and urea plants was indicated by industrial partners involved in the INITIATE project while the overall OPEX is computed according to the methodology reported in [11].

On the other hand, the total plant cost of the MEA post-combustion section installed in the reference ammonia plant is computed according to the bottom-up methodology described in [2] and [10].

3.2.3. INITIATE plants

In the case of the INITIATE plant configurations investigated, a mixed approach is used to compute the total plant cost. The cost of the steel plant without the power section is adapted from [2], the cost of the power plant (considered only for the small-scale) is computed keeping as reference the specific cost per MW of the combined cycle considered in the base case steel plant while the cost of the additional equipment is computed accordingly to the data reported in Table 5. The CAPEX of the SEWGS and of WGS reactors [2] and the cost of the membrane [5], adopted in the large-scale plant only, are adapted from literature.

Table 5: Scaling parameters for equipment purchase cost in Ammonia and INITIATE plants

Plant	Component	Scaling factor	C_0 [M€]	S_0	f
Ammonia	CO_2 capture unit (MEA)	CO_2 mass flow rate, t/h	8.8	12.4	0.6
	CO_2 compressor and condenser	Power, MW	44	50.5	0.67
Initiate	Compressor	Power, MW	8.1	15.3	0.67
	CO_2 compressor and condenser	Power, MW	44	50.5	0.67
	Boiler	Heat duty, MW	0.25	1	0.67
	Pump	Volumetric flow, m^3/h	0.017	250	0.14
	Heat exchanger	Heat transfer, MW	6.1	828	0.67
	WGS	H_2 and CO flow rate, kmol/s	18.34	2.45	0.65
	Methanator	Thermal input, MW_{LHV}	4.77	1246	0.67
	SEWGS single train	Inlet mole flow rate, kmol/s	8.88	1.56	0.67
	Membrane	Inlet $H_2 + N_2$, kmol/h	148.5	3317	0.67

3.3. Key Performance Indicators

The comparison between all the different cases investigated is made through economic and environmental Key Performance Indicators (KPIs) typical of this analysis and available in [2], [5] and [10]. The environmental indexes considered in this study are the Primary Energy Consumption (*PEC*), the specific CO_2 emissions (e_{CO2}), the carbon capture rate (*CCR*), the Specific Primary Energy Consumption for CO_2 Avoided (*SPECCA*) and CO_2 Avoidance (*CA*). The SPECCA indicator is defined as the additional primary energy required (in GJ) to avoid the emission of 1 ton of CO_2 producing the same amount of product. The economic performance is assessed in terms of levelized cost of products, such as Levelized Cost of Hot Rolled Coil, Levelized Cost of Ammonia and Levelized Cost of Urea, and in terms of Cost of CO_2 Avoidance (CCA).

4. Results

The main results of the energy, environmental, and economic assessment are presented in this section.

4.1. Environmental results

The raw material consumption, the CO_2 emissions, the primary energy consumption and the relative KPIs are reported in Table 6 and Fig 1 and Fig 2. Results are computed for two different scenarios. In the first one the electricity imported from the grid has a carbon footprint of 250 kg_{CO2}/MWh while in the second one it is supposed to be from renewable sources, i.e. zero carbon footprint. The PEC related to electricity is considered equal to zero in the renewable scenario since no fossil fuels are consumed.

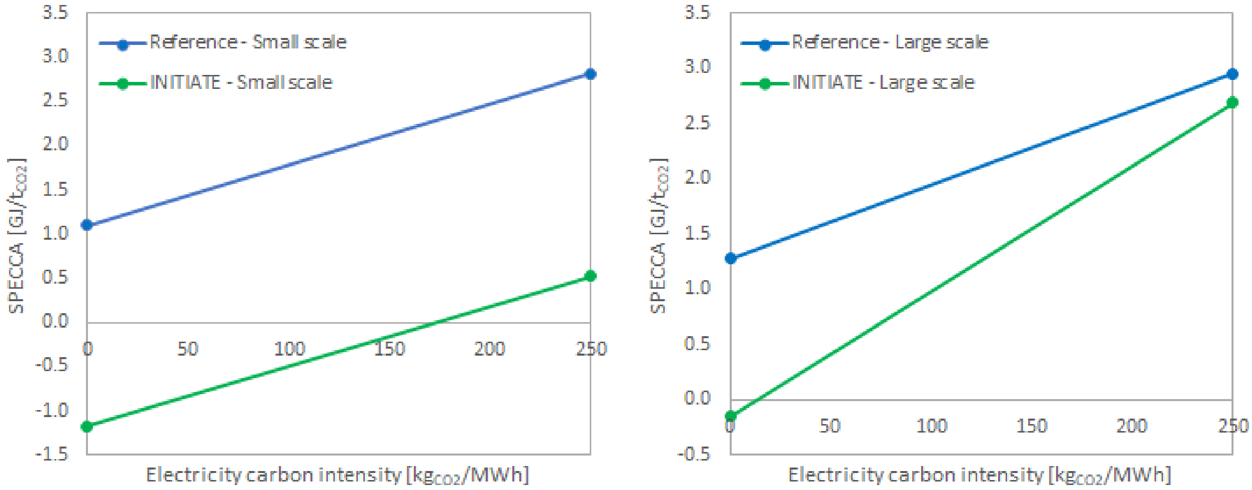

Fig 1: SPECCA vs Electricity carbon intensity for small- and large-scale plants

As can be seen from the graphs, for the range of electricity carbon intensity varying from 0 kg_{CO2}/MWh to 250 kg_{CO2}/MWh, the SPECCA of the INITIATE plants is always lower than the SPECCA of the reference cases. In the case of the small-scale, the SPECCA of the INITIATE plant is lower than the one of the reference case (even for values of electricity carbon intensity higher than 250 kg_{CO2}/MWh) since both the electricity and the natural gas import are higher for the reference case. This is due to the fact that the adoption of the WGS+MDEA carbon capture section in the reference steel mill implies a reduction of the power produced internally but also an increased consumption of natural gas, used to produce the steam necessary for the solvent regeneration. In addition, the symbiotic configuration adopted in the INITIATE allows a further saving of natural gas since ammonia is synthetized starting from BOFG. In the case of the INITIATE large-scale plant, the import of electricity is higher with respect to the base and reference cases but a lower quantity of natural gas is consumed. This happens because in the large-scale configuration all the electricity demand of the steel plant is covered by importing electricity from the grid but also because all the BFG and BOFG available are compressed to the operating pressure of the water gas shift reactor. In addition, the nitrogen present in excess in the BFG contributes in increasing the power consumption of the INITIATE plant, without contributing in the synthesis of ammonia or in other processes. When a low carbon electricity scenario is considered, being the PEC of imported electricity equal or close to zero, the SPECCA indicator becomes even negative, meaning that the symbiotic configuration allows to reduce the primary energy consumption with respect to the base case while reducing the CO_2 emissions.

Furtheremore, the reduction of PEC with respect to the base case is computed for the renewable scenario and excluding the PEC of coal, being the same for all the cases. In the case of the reference cases there is an increase of the PEC equal to 140% and 26.22% while in the case of the INITIATE plants the reduction of PEC is equal to 47% and 8.2% for the small and the large-scale plants respectively.

Table 6: Material import and export of the plants investigated

		Small scale			Large scale		
	Unit	Base case	Reference case	INITIATE	Base case	Reference case	INITIATE
Coal import	t/d	6240.0	6240.0	6240.0	6240.0	6240.0	6240.0
Natural gas import	t/d	92.0	221.1	48.8	602.1	760.0	553.0
Electricity import	MW	7.46	89.0	36.0	2.9	86.0	382.5
Steel production	t/d	9248.8	9248.8	9248.8	9248.8	9248.8	9248.8
Urea production	t/d	224.2	224.2	224.2	1500.0	1500.0	1500.2
CO_2 emissions	t/d	18357	13154	16741	18736	13252	5089

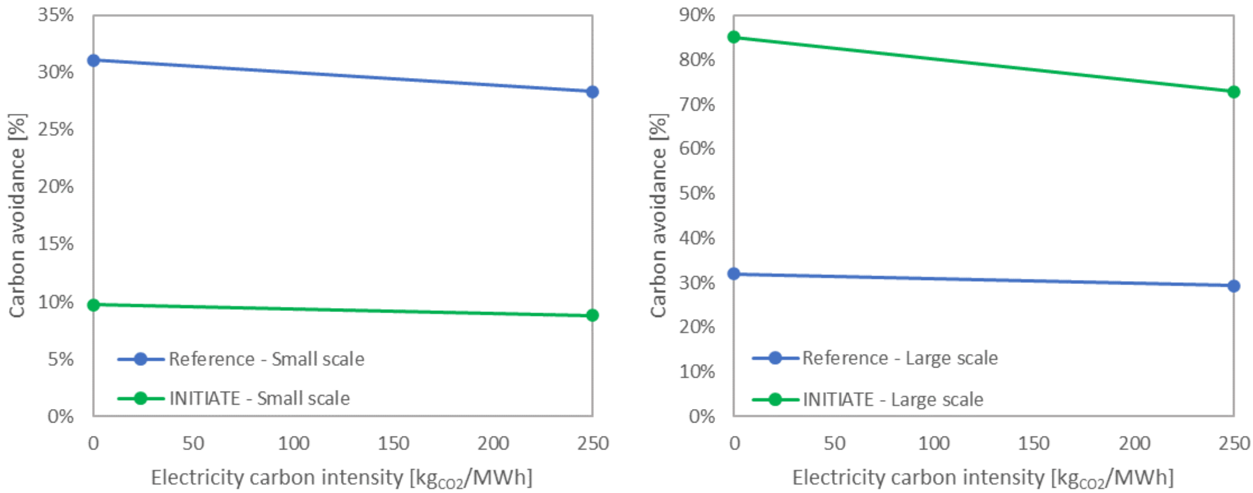

Fig 2: Carbon avoidance vs electricity carbon intensity for small and large scale plants

In Fig 2 the carbon avoidance of the analysed plants is shown. In the case of small-scale INITIATE plant, the reduction of the carbon footprint is limited to 10% since only the BOFG is threated in the WGS+SEWGS section. On the other hand, the large-scale INITIATE plant can achieve a carbon avoidance of 87% when renewable electricity is considered.

4.2. Economic results

The results of the economic analysis are presented in this section. A sensitivity analysis was carried out varying parameters such as the natural gas and the electricity price. The CAPEX of the INITIATE plants is reported in Table 7. As can be observed, the steel plant represents the major contribution along with the membrane that is adopted in the large-scale plant only.

The cost of CO_2 avoided is shown in Fig 3. In every graph only one parameter is varied keeping the others constant. The value used for the analysis are the ones reported in Table 4 considering an electricity carbon footprint equal to 250 kg_{CO2}/MWh.

The results of the sensitivity analysis show an advantage of the small-scale INITIATE plants with respect to the corresponding reference case but also, for certain conditions, with respect to the base plants thanks to the symbiosis between the steel and the urea industries. Indeed, the reduction of the natural gas consumption with respect to both the base and reference cases makes the small-scale INITIATE plants economically advantageous especially in scenarios with a high natural gas price. Furthermore, the industrial symbiosis allows to reduce the carbon footprint but also the annual expenses with respect to the base case, translating in a negative CCA, for a wide range of cases (see Fig 3). In the case of the large-scale plants, the necessity of adopting a membrane, that is a very expensive equipment but also the high electricity consumption, for the above-mentioned reasons, limits the regions in which CCA is lower than CCA of the corresponding reference cases to the ones in which the electricity price is low or the price of natural gas is high. On the other hand, it has to be considered that the carbon avoidance that can be reached with the large-scale INITIATE plant is much higher than the CA of the corresponding reference plants.

Table 7: Capex of small- and large-scale INITIATE plants

Component	Small-scale Capex [M€]	Large-scale Capex [M€]
Gas compressors	22.7	126.2
CO_2 compressor to storage	23.0	143.1
Pumps	0.2	0.2
Heat exchangers	6.4	32.3
Combustors	8.4	25.1
Water gas shifts	3.5	26.7
Methanator	1.6	7.9
Ammonia reactor	5.3	22.5
SEWGS	14.9	213.7
Membrane	0.0	578.8
Steel plant	3869.6	3597.9
Urea plant	96.9	129.6

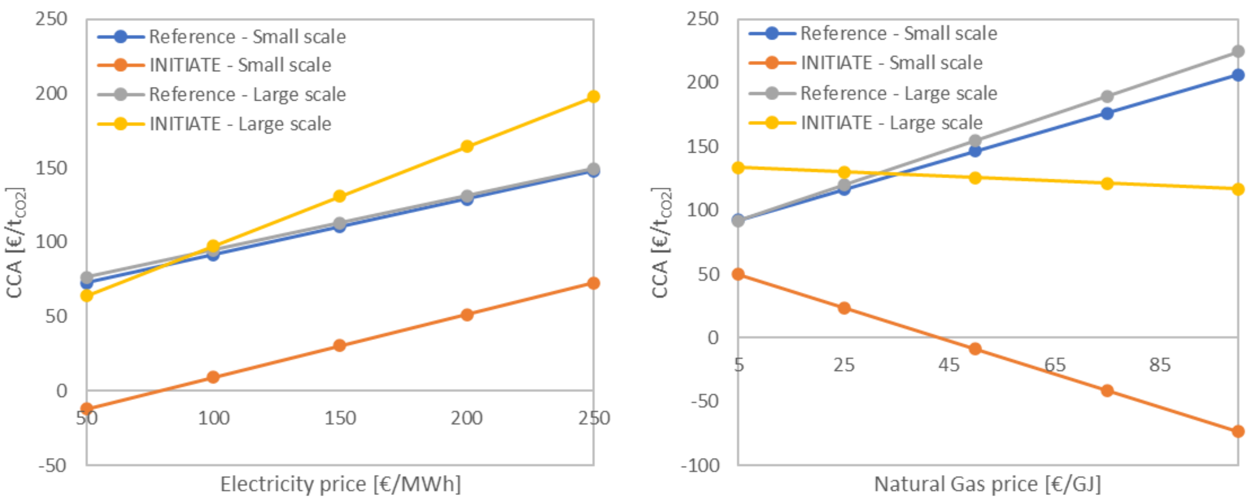

Fig 3: Sensitivity analysis on CCA by varying the electricity price (left) and the NG price (right)

5. Conclusion

This work discusses a preliminary techno-economic assessment of the INITIATE process when integrated with steel plants for CO_2 emissions mitigation and urea production. The analysis is focused on two different urea production capacities. For each investigated plant configuration, costs and performances are assessed and compared to those of the base and reference cases.

The economic and environmental KPIs show a clear advantage of the small-scale INITIATE plant respect to both the base and the reference configuration, result of the industrial symbiosis. On the other hand, the reduction of the carbon footprint is limited to 10%.

The large-scale INITIATE plant can achieve a carbon avoidance of 87% when renewable electricity is considered. This value can be exceeded if instead of natural gas, biofuels are used. Furthermore, for both the sizes, the SPECCA indicator of the INITIATE plants is lower than the SPECCA of the reference plants. By an economic point of view, the cost of CO_2 avoided of the large-scale INITIATE plant is lower than the one of the corresponding reference plants in the case of low electricity prices and high natural gas prices as can be observed in Fig 3.

In general, CCA of the INITIATE plants decreases at a decreasing electricity price and an increasing natural gas cost as a consequence of natural gas savings achieved when the industrial symbiosis is adopted.

In conclusion this works illustrates the advantages that can be obtained environmentally and economically by implementing symbiotic industrial solutions.

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