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Electronic Supplementary Information:

Minimizing CO₂ emissions with renewable energy: A comparative study of emerging technologies in the steel industry

Marian Flores-Granobles and Mark Saeys

S1 Process diagrams of the scenarios



Figure S1. Carbon-based steel mill with power plant. (Scenario 1-CST)



Figure S2. Hydrogen-based steel mill. (Scenario 2-HST)



Figure S3. Carbon-based steel mill with power plant and pre-combustion CO₂ capture using the plant's waste heat. (Scenario 3-CST-WHC)



Figure S4. Carbon-based steel mill with power plant and pre-combustion CO₂ capture using the plant's waste heat and steam from an electric boiler. (Scenario 4-CST-EBC)



Figure S5. Carbon-based steel mill with treatment of the gases originally sent to the power plant, CO₂ storage and methanol production. (Scenario 5-CST-GPP-CCUS)



Figure S6. Carbon-based steel mill with treatment of the gases originally sent to the power plant and burned for heating on site, CO₂ storage and methanol production. (Scenario 6-CST-GPH-CCUS)



Figure S7. Carbon-based steel mill with treatment of the gases originally sent to the power plant, H₂ production by electrolysis and methanol production. (Scenario 7-CST-GPP-CCU)



Figure S8. Carbon-based steel mill with treatment of the gases originally sent to the power plant and burned for heating on site, H₂ production by electrolysis and methanol production. (Scenario 8-CST-GPH-CCU)



S2 Effect of the Grid Emission Intensity (GEI) on the CO₂ emissions for the different scenarios

Figure S9. Sensitivity of the CO₂ emissions for the different scenarios on the Grid Emission Intensity (GEI).

S3 CO₂ stored and methanol produced in the scenarios

Scenario	CO ₂ Stored [t CO ₂ /t l.s.]	Methanol Produced [t methanol/t l.s.]
2 HST	0	0
3 CST-WHC	0.02	0
4 CST-EBC	0.34	0
5 CST-GPP-CCUS	0.63	0.14
6 CST-GPH-CCUS	1.0	0.22
7 CST-GPP-CCU	0	0.59
8 CST-GPH-CCU	0	0.96

Table S1. CO₂ stored and methanol produced in the scenarios

S4 Data for the scenarios

Description	Value	Units	Source
Feedstock for the steel plant	14	GJ/t l.s.	Gross and net fuel input for the hot metal production of a conventional steel plant ¹ .
Feedstock for heating in the steel plant	3.2	GJ/t l.s.	Own calculation based on the replacement of the steel mill gases with natural gas ¹
Waste heat from the steel plant available for amine scrubbing	-0.047	GJ/t l.s.	Waste heat over 150 °C ^{2, 3}
Electricity required at the steel plant	0.23	MWh/t l.s.	Electricity consumption of a conventional steel plant ¹ .
Electricity generated in the power plant	-0.45	MWh/t l.s	Own calculation based on the composition of the gases sent to the power plant and a 32.1% of thermal efficiency ¹ .
CO ₂ emissions from the steel plant (not-related to electricity)	1.0	t CO ₂ /t l.s.	Includes the CO ₂ emissions from the pellet plant ⁴ , sinter plant, lime plant, the combustion of part of the steel mill gases to generate heat in the plant and flared gases ¹ .
CO ₂ emissions from the use of natural gas as heating in the plant	0.18	t CO ₂ /t I.s.	Own calculation based on the composition of the natural gas pipeline available in the steel plant ¹ .
CO_2 emissions from the power plant	0.93	t CO₂/t I.s.	Own calculations based on the composition of the gases sent to the power plant in a conventional steel plant ¹ .

Table S2. Data for the conventional steel plant

Table S3. Data for the capture of CO_2 from the pre-combustion BFG.

Description	Value	Units	Source
			Modelled values in Aspen Plus based on the
Electricity for the amine scrubber	0.22	MWh/t CO ₂	compression of BFG to 6 bar ³ and the compression of CO_2 to 110 bar ¹ .
Electricity required for the electric boilers	0.29	MWh/t l.s.	Own calculation based on 2.4 GJ/t CO _{2 captured} are required at 150 °C ³ and an efficiency of 97% of the electric boilers ⁵ .

Description	Value	Units	Source
Coal in the EAF	0.85	GJ/t l.s.	Input of 27 kg of coal in the EAF (31.1 MJ/kg coal ¹), considering that half of the carbon stays in the steel and the other half is emitted as 50 kg CO ₂ /t l.s. ⁶ .
Electricity required at the direct reduction plant and EAF	0.63	MWh/t l.s.	Based on literature ⁷ .
Electricity required for the production of H_2 .	3.6	MWh/t l.s	Own calculation based on 94% of metallization ⁷ (1.06 t DRI/t l.s.), 8.2 GJ/t DRI of hydrogen ^{6, 8} and 4.5 kWh/Nm ³ H ₂ ⁹ .
CO ₂ emissions from pellet production	0.12	t CO ₂ /t l.s.	Based on literature ⁴
CO ₂ emissions from carbon addition to the EAF	0.050	t CO ₂ /t l.s.	Based on literature ⁶
CO ₂ emissions from lime production	0.056	t CO ₂ /t l.s.	Based on literature ¹
CO ₂ emissions from the decomposition of the electrodes in the EAF	0.0070	t CO₂/t I.s.	Based on literature ¹⁰

Table S4. Collected data for the ${\rm H_2}\textsc{-}based$ steel plant

Table S5. Data for conventional methanol production

Description	Value	Units	Source
Feedstock for the fossil methanol production	25	GJ/t methanol	Natural gas⁵.
Fuel for the fossil methanol production	14	GJ/t methanol	Natural gas⁵.
Steam exported from the methanol production	-2.0	GJ/t methanol	Based on literature⁵.
Direct CO ₂ emissions from the steel plant (not-related to electricity)	0.52	t CO_2 /t methanol	Based on literature ⁵ .

Description	Value	Units	Source
Electricity for alternative methanol synthesis	1.5	MWh/t methanol	Based on literature⁵.
Electricity for the PSA unit	GPP: 0.015 GPH: 0.027	MWh/t l.s.	Process modelling based on the composition of the COG ¹ and a recent patent for the recovery of 90% of the H_2^{11} .
Electricity for the SEWGS process	GPP: 0.29 GPH: 0.46	MWh/t l.s.	Process modelling based on the composition of the BFG and BOFG ¹ , gas compression to 26 bar ¹² , the compression of the H ₂ -rich gas for the 2-stages membrane separation ¹³ and the electrical requirement of the steam boilers with 97% of efficiency ⁵
CO_2 emissions from the combustion of the N_2 -rich gas after membrane separation	GPP: 0.048 GPH: 0.077	t CO ₂ /t l.s.	Process modelling based on the composition of BFG and BOFG ¹ and the 2-stages membrane separation ¹³
Electricity for the production of H_2	4.5	kWh/Nm ³ H ₂	Based on literature ⁹ .

Table S6. Data for alternative methanol production

Table S7. Electricity requirements

Scenario	Steel Mill [MWh/t l.s.]	Carbon Storage [MWh/t l.s.]	Alternative Methanol Plant [MWh/t l.s.]	Electrolyzer [MWh/t l.s.]	Total [MWh/t l.s.]
1 CST	-0.22	-	-	-	-0.22
2 HST	4.2	-	-	-	4.2
3 CST-WHC	-0.22	0.0043	-	-	-0.22
4 CST-EBC	-0.22	0.36	-	-	0.14
5 CST-GPP-CCUS	0.20	0.078	0.51	-	0.79
6 CST-GPH-CCUS	0.19	0.13	0.82	-	1.1
7 CST-GPP-CCU	0.13	-	1.2	4.2	5.6
8	0.064	-	1.9	6.9	8.9

CST-GPH-CCU

$S5\ CO_2$ emissions in the scenarios

Scenario	Steel Mill [t CO ₂ /t l.s.]	CO ₂ capture and storage [t CO ₂ /t l.s.]	Alternative Methanol Plant [t CO ₂ /t l.s.]	Electrolyzer [t CO ₂ /t l.s.]	Total [t CO ₂ /t l.s.]
1 CST	1.9	-	-	-	1.9
2 HST	0.4	-	-	0.9	1.3
3 CST-WHC	1.9	0.0011	-	-	1.9
4 CST-EBC	1.6	0.036	-	-	1.6
5 CST-GPP-CCUS	0.99	0.020	0.17	-	1.2
6 CST-GPH-CCUS	0.55	0.03	0.28	-	0.86
7 CST-GPP-CCU	0.75	-	0.35	1.1	2.2
8 CST-GPH-CCU	0.17	-	0.56	1.7	2.4

Table S8. CO_2 emissions in the scenarios with a $GEI_1 = 0.25$ t CO_2/MWh

Table S9. CO_2 emissions in the scenarios with a $GEI_2 = 0.01 \text{ t } CO_2/\text{t } MWh$

Scenario	Steel Mill [t CO ₂ /t l.s.]	CO ₂ capture and storage [t CO ₂ /t l.s.]	Alternative Methanol Plant [t CO ₂ /t l.s.]	Electrolyzer [t CO ₂ /t l.s.]	Total [t CO ₂ /t l.s.]
1 CST	1.9	-	-	-	1.9
2 HST	0.25	-	-	0.040	0.29
3 CST-WHC	1.9	0.000047	-	-	1.9
4 CST-EBC	1.6	0.0016	-	-	1.6
5 CST-GPP-CCUS	0.93	0.00086	0.053	-	0.99
6 CST-GPH-CCUS	0.49	0.0014	0.086	-	0.58
7 CST-GPP-CCU	0.70	-	0.061	0.047	0.80
8 CST-GPH-CCU	0.11	-	0.098	0.076	0.29

S6 Efficiency of the use of energy for the reduction of CO₂ emissions in the scenarios

Scenario	GEI ₁ = 0.25 t CO _{2 emitted} /MWh _{produced} [MWh _{consumed} /t CO _{2 captured}]	GEI ₂ = 0.01 t CO _{2 emitted} /MWh _{produced} [MWh _{consumed} /t CO _{2 captured}]
2 HST	7.1	2.7
3 CST-WHC	-	-
4 CST-EBC	0.5	0.4
5 CST-GPP-CCUS	1.3	1.1
6 CST-GPH-CCUS	1.3	1.0
7 CST-GPP-CCU	-	5.1
8 CST-GPH-CCU	-	5.5

Table S10: Electricity consumed per CO₂ removed.

S7 Methodology for mass and energy balances of the scenarios 1-CST, 2-HST and 8-CST-GPH-CCU.

A. 1-CST

A reference integrated steel mill was selected from a study by the International Energy Agency (IEA)¹. The mass and energy balances correspond to the production of 1 ton of liquid steel from the Basic Oxygen Furnace. Hence, the ladle metallurgy, continuous casting and rolling sections were not considered in this analysis. A detailed description of the steel mill's off gases is shown in Table 1. Part of the gases is used to generate heat in the steel production process and another part is sent to the power plant to generate 450 kWh/t l.s. of electricity, see Figure S10. The electricity required by the steel mill is 230 kWh/t l.s., indicating that the power plant produces more electricity than required by the steel plant.

B. 2-HST

The mass and energy balances of a H_2 -based steel plant were performed with the information given in Table S4. All the data was collected from literature and the balances were performed as shown in Figure 11.

C. 8-CST-GPH-CCU

The reference steel mill 1-CST is used as the base for the calculation of this scenario. All the steel mill gases were sent to the gas treatment plant and natural gas was used to generate the heat required in the steel plant; this calculation is shown in Figure S12. The mass balances and electricity requirements of the gas treatment plant were calculated with Aspen Plus, Matlab and data collected from literature as presented in Tables S2, S5 and S6. A summary of the calculations is displayed in Figures S12 and S13.

In the gas treatment plant, 90% of H_2 from COG was recovered via PSA and the CH₄-rich stream was exported to a natural-gas-consuming plant, hence the CO₂ emitted by combusting this stream was avoided by the steel plant. In scenario 1-CST, this CH₄ is combusted in the power plant.

The BFG and BOFG were sent to a SEWGS process where additional steam was used to transform CO into H_2 and CO_2 while simultaneously separating the CO_2 -rich and H_2 -rich streams. The process was modeled in Aspen Plus to recover 95% of the CO_2 in the CO_2 -rich stream at 95% purity. The H_2 -rich stream contains most of the N_2 , which was then separated by a 2-stage H_2/N_2 separation using polymeric membranes. The heat requirements of the SEWGS process were supplied by combustion of the N_2 -rich stream after membrane separation and by electric boilers.

The mass balance for the membrane separation was calculated considering the permeance of the gases, solving the equation systems with Matlab and implementing the resulting gas composition from each stage in the Aspen Plus model for the SEWGS process. In the membranes section, the gas was at 26 bar for the first separation stage, the outlet pressure was at 2 bar for 97% H₂ recovery and an area of 230 m². For the second stage, the gas was recompressed to 9 bar before flowing through the second membrane with 210 m² of area, so 90% of the H₂ entering the separation section was recovered at 1 bar. The N₂-rich gas contained 10% of the H₂ and was combusted to recover heat for the SEWGS process. The methanol plant was modelled in Aspen Plus to validate the data from literature. An overview of the methanol synthesis loop flowsheet is shown in Figure S14.

1-CST Steel plant

Section	COG [Nm³/t l.s.]	BFG [Nm³/t l.s.]	BOFG [Nm³/t l.s.]	Electricity consumption [kWh/t l.s.]	Steam consumption [kg/t l.s.]	CO ₂ emissions [t CO ₂ /t l.s.]
Coke production	123	-170	0	13	57	0.18
Sinter and pellets production	-4.3	0	0	33	0	0.30
Hot metal production	-8.0	1028	0	95	7.3	0.41
Crude steel production	0	0	82	20	-71	0.047
Lime production	-16	0	0	2.4	0	0.067
Oxygen production	0	0	0	62	6.8	0
Total	95	858	82	226	0.0	1.0
	Gases se	nt to the nov	ver plant			

Gases sent to the power plant

Power plant

Component	From COG [Nm³/t l.s.]		From BOFG [Nm³/t l.s.]	Total [Nm³/t l.s.]	LHV [MJ/Nm³]	[MJ/t l.s.]	CO ₂ emissions [t CO ₂ /t l.s.]
CH₄	21.9	0	0	21.9	36	785	0.043
H ₂	56.6	31.1	2.2	89.9	11	972	0
СО	3.7	191.6	46.6	241.8	13	3073	0.47
CO2	0.9	189.6	11.8	202.3	0	0	0.40
Other HC (CxHy)	2.6	0	0	2.6	63	162	0.010
					Total [MJ/t l.s.]	4992	0.92

Considering 32.1% efficiency in the power plant:	
Electricity produced:	1603 MJ/t l.s.
Electricity produced:	445 kWh/t l.s.
Carbon intensity of the electricity:	2.1 t CO ₂ /MWh

Summary

Section	Electricity consumption [MWh/t l.s.]	Non-related to electricity CO2 emissions [t CO2 /t l.s.]
Steel plant	226	1.0
Power plant	-445	0.92
Total	-220	1.9

Figure S10. Methodology for mass and energy balances of the scenario 1-CST.

2-HST Steel plant

			Ref.
Energy consumption for Direct Reduction with 100% H ₂ in ENERGIRON plants	8.2	GJ H ₂ /t DRI	8
Lower Heating Value H₂	0.011	GJ H ₂ /Nm ³	
Metallization	94	%	7
t DRI/t l.s. ratio based in metallization	1.1	t DRI/t l.s.	
Electricity for H ₂ production in electrolyzers	4.5	kWh/Nm ³	9
Electricity required for H ₂ production	3.6	MWh/t l.s.	

$\frac{8.2 GJ H_2}{t DRI} \cdot \frac{Nm^3 H_2}{0.011 GJ H_2} \cdot \frac{t DRI}{0.94 t l.s.} \cdot \frac{4.5 kWh}{Nm^3 H_2} \cdot \frac{MWh}{1000 kWh} = 3.6 \frac{MWh}{t l.s.}$

Section	Electricity consumption [MWh/t l.s.]	Non-related to electricity CO ₂ emissions [t CO ₂ /t l.s.]	Ref.
Pellet production	-	0.13	4
Lime production	0.002	0.056	1
Electricity for H ₂ production	3.6	Depends on GEI	6
Carbon addition in EAF	-	0.05	6
Electricity for EAF	0.63	Depends on GEI	7
Decomposition electrodes in EAF	-	0.007	10
Total	4.2	0.24	3

Total emissions when GEI = 0.25 t CO ₂ /MWh	1.3	t CO ₂ /t l.s.
Total emissions when GEI = 0.01 t CO ₂ /MWh	0.29	t CO ₂ /t l.s.

Figure S11. Methodology for mass and energy balances of the scenario 2-HST.

8-CST-GPH-CCU Steel, gas treatment and methanol plants.

Steel plant:

Section	COG [Nm³/t l.s.]	BFG [Nm³/t l.s.]	BOFG [Nm³/t l.s.]	Electricity consumption [kWh/t l.s.]	Natural gas consumption [MJ/t l.s.]	Steam consumption [kg/t l.s.]	CO ₂ emissions [t CO ₂ /t l.s.]
Coke production	166	0	0	13.2	1280.2	56.5	0.077
Sinter and pellets production	0	0	0	32.9	74.5	0	0.30
Hot metal production	0	1467	0	95.2	1545.5	7.3	0.11
Crude steel production	0	0	81.8	20.0	0	-70.6	0.046
Lime production	0	0	0	2.4	277.3	0	0.072
Oxygen production	0	0	0	61.8	0	6.8	0
Total	166	1467	82	226	3178	0.0	0.60
8	Gases sen	t to gas treatm	nent plant	8	78	Nm ³ NG/t l.s.	

Gas treatment plant - PSA (literature and Aspen Plus)

Component	COG in [Nm³/t l.s.]	COG in [kmol/t l.s.]	H ₂ rich gas [kmol/t l.s.]	PSA off-gas [kmol/t l.s.]	LHV [MJ/Nm³]	[MJ/t l.s.]	
CH₄	38	1.7	0.0	1.7	36	1369	
H ₂	99	4.4	4.0	0.44	11	107	
со	6.4	0.28	0.0	0.28	13	81	
CO ₂	1.6	0.071	0.0	0.07	0	0	
Nz	9.6	0.43	0.0	0.43	0	0	
02	0.32	0.014	0.0	0.014	0	0	
H ₂ O	6.6	0.29	0.0	0.29	0	0	Exported to a natura
Other HC (CxHy)	4.5	0.20	0.0	0.20	63	282	gas consuming plant
		,	to methanol plant		Total [MJ/t l.s.]	1838	24 MJ/Nm ³

Figure S12. Methodology for mass and energy balances of the scenario 8-CST-GPH-CCU (part A).

Gas treatment plant - SEWGS (Aspen Plus)

Component	(dry basis)	BFG+BOFG in (dry basis) [kmol/t l.s.]	After SEWGS (dry basis) CO ₂ rich gas [kmol/t l.s.]	After SEWGS (dry basis) H ₂ rich gas [kmol/t l.s.]
H ₂	55	2.5	0.59	18
со	373	17	0.013	0.39
CO2	334	15	30	1.6
Nz	723	32	1.0	31
			to methanol plant	to H_2/N_2 separation

Gas treatment plant - H₂/N₂ separation (Matlab)

Component	After SEWGS in (dry basis) [kmol/t l.s.]	H2 rich gas out of 1st membrane (dry basis) [kmol/t l.s.]	H₂ rich gas out of 2nd membrane (dry basis) [kmol/t l.s.]	H ₂ lean gas out of H ₂ /N ₂ separation (dry basis) [kmol/t l.s.]
H ₂	18	18	16	1.8
со	0.39	0.012	0.003	0.39
CO ₂	1.6	0.52	0.16	1.4
N ₂	31	0.54	0.008	31
	201	to 2nd membrane	to methanol plant	Burned for energy recovery

0.08 t CO₂/t l.s. Emissions

Methanol plant (literature and Aspen Plus)

Component	H ₂ rich gas from PSA (dry basis) [kmol/t l.s.]	CO2 rich gas from SEWGS (dry basis) [kmol/t l.s.]	H₂ rich gas from H₂/N₂ separation (dry basis) [kmol/t l.s.]	H₂ from electrolyzer[kmol/t l.s.]
H ₂	4.0	0.59	16	68
со	0.0	0.013	0.003	0.0
CO ₂	0.0	30	0.16	0.0
N ₂	0.0	1.0	0.008	0.0

Methanol produced	0.96 t methanol/t l.s.
Electricity for methanol production	1.5 MWh/t methanol
Electricity required	1.4 MWh/tl.s.

Replacement of conventi	onal methanol:
Electricity credit	-0.16 kWh/t l.s.
CO ₂ credit	-0.50 t CO ₂ /t l.s.

Electrolyzer

H₂ required	1534 Nm ³ /t l.s.
Electrity in the electrolyzer	4.5 kWh/Nm ³
Electricity required	6.9 MWh/tl.s

Summary

Section	Electricity consumption [MWh/t l.s.]	Non-related to electricity CO ₂ emissions [t CO ₂ /t l.s.]	
Steel plant	0.23	0.61	Total emissions when:
PSA	0.027	0	GEI = 0.25 t CO ₂ /MWh
SEWGS + H ₂ /N ₂ separation	0.46	0.079	2.4 t CO ₂ /t l.s.
Methanol plant	1.4	0	
Electrolyzer	6.9	0	$GEI = 0.01 t CO_2/MWh$
Replacement of conventional methanol synthesis	-0.16	-0.50	0.29 t CO2/t l.s.
Total	8.9	0.19	

Figure S13. Methodology for mass and energy balances of the scenario 8-CST-GPH-CCU (part B).



Figure S14. Methanol synthesis loop section of the Aspen Plus validation model.

S8 Selected values and sensitivity analysis of key process variables.

Variable	Selected Value	Range	Source
Power plant efficiency	32.1%	-	Based on literature ¹ .
H ₂ required in the H ₂ -based steel-making	8.2 GJ H ₂ /t DRI	-	Based on literature ⁶ .
DRI metallization	94%	94-96%	Based on literature ⁷ .
Power in electrolyzer	4.5 kWh/Nm³	3.2 – 6.1 kWh/Nm ³	Based on literature ^{6, 9} .
Power in EAF	630 kWh/t l.s.	Cold DRI: ~670 kWh/t l.s. Hot DRI: ~580 kWh/t l.s.	Based on literature ⁷ .
H ₂ recovery after PSA	90%	70-90%	Based on literature ¹¹ and PSA provider.
SEWGS	CO_2 capture: 95% CO_2 purity: 95%	Latest campaign: CO2 capture > 90% CO2 purity > 90%	Based on their latest campaign ¹⁴ .
Methanol synthesis	100% gas conversion	Reached 100% with the lowest purge.	Based on literature ⁵ and confirmed with Aspen Plus model.





Figure S15. Sensitivity analysis for 3 key performance parameters for CCUS scenario 6 using electricity from a mixed and a renewable grid.



Figure S16. Sensitivity analysis for 3 key process performance parameters for CCU scenario 8 using electricity from a mixed and a renewable grid.

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