Electronic Supplementary Material (ESI) for Energy & Environmental Science.

Supplementary Information

Green steel: design and cost analysis of hydrogen-based direct iron reduction

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S1. State-point stream data

Table S1: State-point stream data for the NG-DRI-B case

Stream Number	Unit	1	2	3	4	5	6	7	8	9
Temperature	°C	25	850	466	25	66	500	433	25	500
Pressure	bar	2.0	2.7	1.7	4.0	1.6	1.1	0.9	4.0	2.9
Mole Flowrate	kmol/h	1,436	11,143	11,204	323	3,356	8,633	11,089	1,399	8,477
Mass Flowrate	kg/h	216,134	163,566	221,313	5,175	65,653	248,268	313,921	22,450	163,566
Molar Vapor Fraction	–	0	1	1	1	1	1	1	1	1
Composition	mole-basis									
O_2	–	0	0	0	0	0	0.208	0.022	0	0
N_2	–	0	0	0	0	0	0.783	0.610	0	0
H_2O	–	0	0.084	0.263	0	0.165	0.008	0.219	0	0.153
H_2	–	0	0.510	0.339	0	0.340	0	0	0	0.314
CH_4	–	0	0.007	0.002	1	0.098	0	0	1.000	0.167
CO	–	0	0.345	0.196	0	0.196	0	0	0	0.181
CO_2	–	0	0.053	0.200	0	0.200	0	0.150	0	0.185
Fe_2O_3	–	0.895	0	0	0	0	0	0	0	0
Al_2O_3	–	0.030	0	0	0	0	0	0	0	0
SiO_2	–	0.075	0	0	0	0	0	0	0	0
Fe	–	0	0	0	0	0	0	0	0	0
C	–	0	0	0	0	0	0	0	0	0
Total	–	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream Number	Unit	10	11	12	13	14	15	16	17
Temperature	°C	700	148	148	25	25	25	925	1650
Pressure	bar	2.0	10.0	10.0	4.0	1.0	1.0	1.0	1.0
Mole Flowrate	kmol/h	2,705	15	233	60	310	–	1,545	2,485
Mass Flowrate	kg/h	158,849	467	7,392	957	3,723	6,791	45,449	135,812
Molar Vapor Fraction	–	0	1	1	1	0	0	1	0
Composition	mole-basis								
O_2	–	0	0.945	0.945	0	0	0	0.087	0
N_2	–	0	0.055	0.055	0	0	0	0.602	0
H_2O	–	0	0	0	0	0	0	0.077	0
H_2	–	0	0	0	0	0	0	0	0
CH_4	–	0	0	0	1.000	0	0	0	0
CO	–	0	0	0	0	0	0	0.119	0
CO_2	–	0	0	0	0	0	0	0.115	0
Fe_2O_3	–	0.029	0	0	0	0	0	0	0
Al_2O_3	–	0.016	0	0	0	0	0	0	0
SiO_2	–	0.040	0	0	0	0	0	0	0
Fe	–	0.894	0	0	0	0	0	0	0.973
C	–	0.022	0	0	0	1.000	0	0	0.027
Total	–	1.000	1.000	1.000	1.000	1.000	0	1.000	1.000

Table S2: State-point stream data for the H_2-DRI-B case

Stream Number	Unit	1	2	3	4	5	6	7	8	9
Temperature	°C	25	775	351	25	41	28	221	25	55
Pressure	bar	2.0	2.6	1.7	4.0	1.6	1.0	1.0	35.0	2.8
Mole Flowrate	kmol/h	1,436	6,134	6,149	102	402	1,956	2,225	4,407	6,134
Mass Flowrate	kg/h	216,142	16,407	83,088	1,630	2,937	56,035	58,972	8,884	16,407
Molar Vapor Fraction	–	0	1	1	1	1	1	1	1	1
Composition	mole-basis									
O_2	–	0	0	0	0	0	0.206	0.030	0	0
N_2	–	0	0.014	0.016	0	0.037	0.775	0.688	0	0.014
H_2O	–	0	0.019	0.692	0	0.049	0.019	0.236	0	0.019
H_2	–	0	0.968	0.292	0	0.661	0	0	1.000	0.968
CH_4	–	0	0	0	1.000	0.253	0	0	0	0
CO	–	0	0	0	0	0	0	0	0	0
CO_2	–	0	0	0	0	0	0	0.046	0	0
Fe_2O_3	–	0.895	0	0	0	0	0	0	0	0
Al_2O_3	–	0.030	0	0	0	0	0	0	0	0
SiO_2	–	0.075	0	0	0	0	0	0	0	0
Fe	–	0	0	0	0	0	0	0	0	0
C	–	0	0	0	0	0	0	0	0	0
Total	–	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Stream Number	Unit	10	11	12	13	14	15	16	17
Temperature	°C	700	148	148	25	25	25	925	1650
Pressure	bar	2.0	10.0	10.0	4.0	1.0	1.0	1.0	1.0
Mole Flowrate	kmol/h	2,645	273	233	13	375	–	1,545	2,485
Mass Flowrate	kg/h	158,127	8,666	7,393	216	4,504	6,791	45,454	135,817
Molar Vapor Fraction	–	0	1	1	1	0	0	1	0
Composition	mole-basis								
O_2	–	0	0.945	0.945	0	0	0	0.083	0
N_2	–	0	0.055	0.055	0	0	0	0.600	0
H_2O	–	0	0	0	0	0	0	0.079	0
H_2	–	0	0	0	0	0	0	0	0
CH_4	–	0	0	0	1.000	0	0	0	0
CO	–	0	0	0	0	0	0	0.121	0
CO_2	–	0	0	0	0	0	0	0.117	0
Fe_2O_3	–	0.029	0	0	0	0	0	0	0
Al_2O_3	–	0.016	0	0	0	0	0	0	0
SiO_2	–	0.041	0	0	0	0	0	0	0
Fe	–	0.914	0	0	0	0	0	0	0.973
C	–	0	0	0	0	1.000	0	0	0.027
Total	–	1.000	1.000	1.000	1.000	1.000	0	1.000	1.000

S2. EAF off-gas profiles

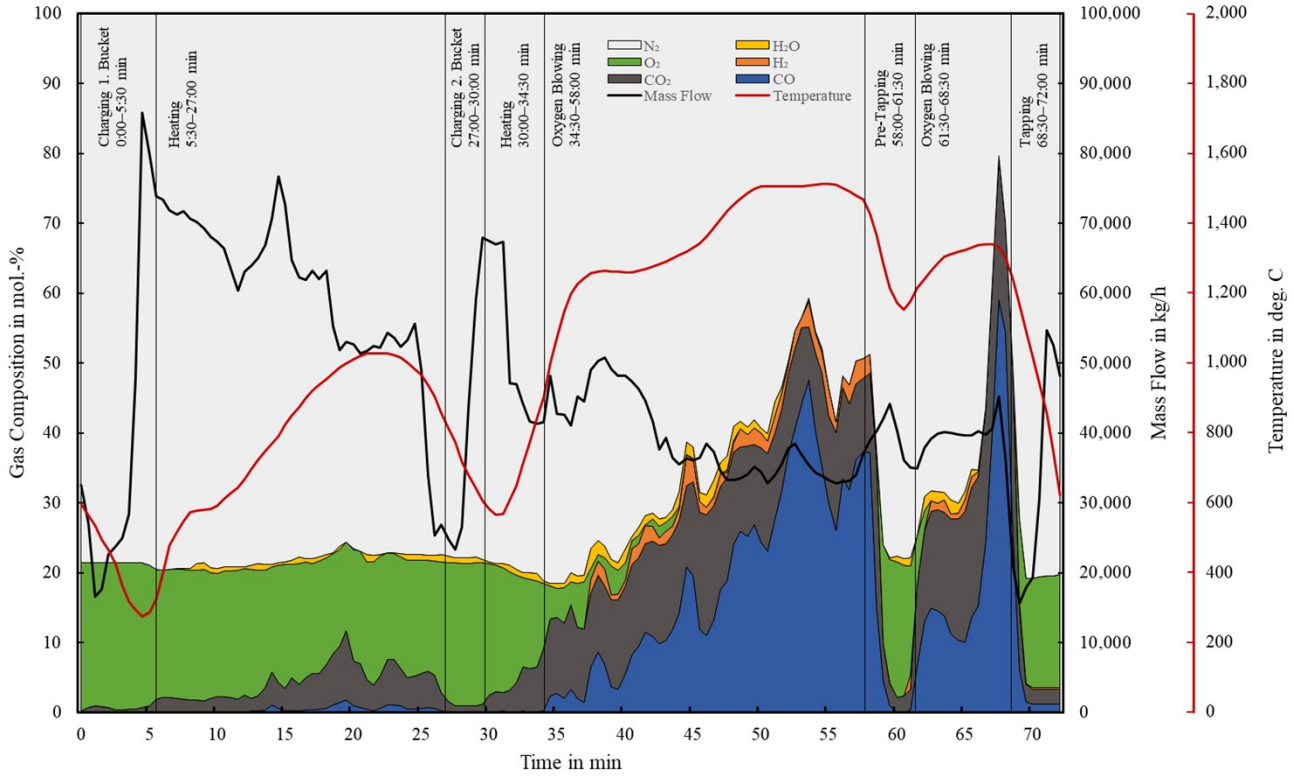

Figure S1: EAF off-gas #1 composition, temperature, and mass flow profiles. Adapted from [1].

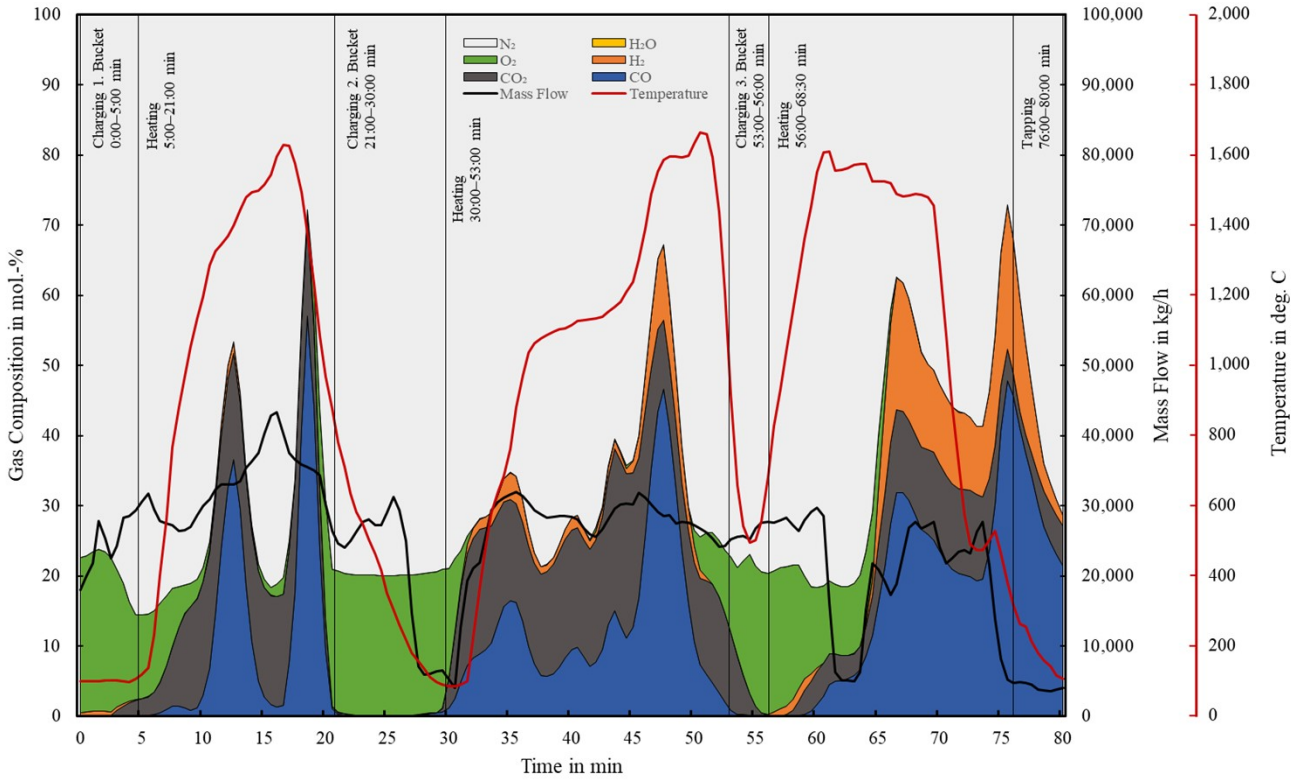

Figure S2: EAF off-gas #2 composition, temperature, and mass flow profiles. Adapted from [2].

S3. Performance summary NG-DRI-B case

Table S3: Steel Plant Performance for the NG-DRI-B Case

Plant Design Capacity	Value	Unit
Steel Slab Production Capacity	1,162,120	metric tonnes/year
Plant Capacity Factor	90	%
Actual Steel Slab Production	1,045,908	metric tonnes/year
Consumables at 90% CF	**Value**	**Unit**
Iron Ore Pellets	1,704,001	metric tonnes/year
Natural Gas	11,359,188	GJ/year
Electricity	606,461	MWh/year
Carbon	29,355	metric tonnes/year
Lime	53,537	metric tonnes/year
Raw Water Withdrawal	1,336,953	metric tonnes/year
Emissions at 90% CF	**Value**	**Unit**
Direct Carbon Dioxide Emissions	706,351	metric tonnes/year
Specific Direct CO_2 Emission	0.675	kg_{CO2}/kg_{Steel}
Specific Indirect CO_2 Emission	0.643	kg_{CO2}/kg_{Steel}
Slag	182,329	metric tonnes/year
Surface Water Discharge	372,889	metric tonnes/year

Table S4: Steel Plant Energy Balance for the NG-DRI-B Case at Full Capacity

Energy Output	Value	Unit
Steel Chemical Energy, 0.6%-C (LHV)	277,546	kW
Energy Input	**Value**	**Unit**
Methane Chemical Energy (LHV)	400,219	kW
Carbon Chemical Energy (LHV)	33,886	kW
Reformer Furnace Air Blower	1,284	kW
Process Gas Recycle	5,367	kW
Stack Air Blower	3,738	kW
Scrubber Water Circulation Pump	134	kW
Cooling Tower Fans	175	kW
Cooling Tower Water Circulation Pump	757	kW
Oxygen PSA	5,249	kW
EAF Reactor	48,162	kW
EAF Induced Draft Fan	165	kW
Ladle Refining	3,657	kW
Miscellaneous Balance of Plant	8,236	kW
Energy Efficiency	**Value**	**Unit**
Steel Reduction Thermal Efficiency	54.31	%

Table S5: Steel Plant Economics for the NG-DRI-B Case

Overnight Cost	Value	Unit
Total Plant Cost	795,535	$ (thousands)
Preproduction Cost	90,334	$ (thousands)
Inventory Capital Cost	46,646	$ (thousands)
Initial Catalyst, Sorbent & Chemicals Cost	307	$ (thousands)
Land	900	$ (thousands)
Other Owners' Costs (18.4% of TPC)	119,330	$ (thousands)
Financing Costs	21,479	$ (thousands)
Fixed Operating Cost	**Value**	**Unit**
Annual Labor Cost	94,713	$ (thousands)
Annual Tax and Insurance Cost	15,911	$ (thousands)
Variable Operating Cost	**Value**	**Unit**
Annual Iron Ore Pellet Feedstock Cost	221,520	$ (thousands)
Annual Natural Gas Cost	106,803	$ (thousands)
Annual Electricity Cost	56,643	$ (thousands)
Annual Maintenance Materials Cost	10,695	$ (thousands)
Annual Chemical, Catalyst & Disposal Costs	19,238	$ (thousands)
Economic Performance Metrics	**Value**	**Unit**
Specific Steel Plant Cost	669	$/metric tonne steel
1st Year Levelized Cost of Steel	582.18	$/metric tonne steel

S4. Performance summary H_2-DRI-B case

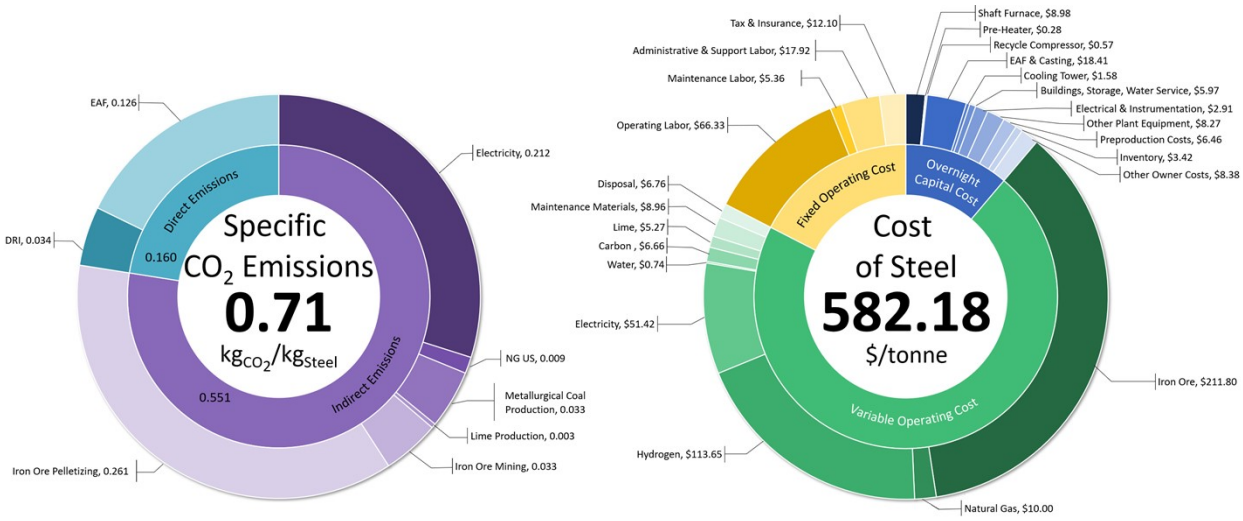

Figure S3: Breakdown of carbon dioxide emissions (left) and levelized cost of steel (right) for the H_2-DRI-B case.

Table S6: Steel Plant Performance for the H_2-DRI-B Case

Plant Design Capacity	Value	Unit
Steel Slab Production Capacity	1,162,120	metric tonnes/year
Plant Capacity Factor	90	%
Actual Steel Slab Production	1,045,908	metric tonnes/year
Consumables at 90% CF	**Value**	**Unit**
Iron Ore Pellets	1,704,063	metric tonnes/year
Hydrogen Gas	70,042	metric tonnes/year
Natural Gas	1,111,997	GJ/year
Electricity	575,773	MWh/year
Carbon	35,511	metric tonnes/year
Lime	53,537	metric tonnes/year
Raw Water Withdrawal	1,259,784	metric tonnes/year
Emissions at 90% CF	**Value**	**Unit**
Direct Carbon Dioxide Emissions	167,487	metric tonnes/year
Specific Direct CO_2 Emission	0.160	kg_{CO2}/kg_{Steel}
Specific Indirect CO_2 Emission	0.551 (0.581)*	kg_{CO2}/kg_{Steel}
Slag	182,335	metric tonnes/year
Surface Water Discharge	458,743	metric tonnes/year

*Considering an emission factor of 0.45 kg_{CO2}/kg_{H2}

Table S7: Steel Plant Energy Balance for the H_2-DRI-B Case at Full Capacity

Energy Output	Value	Unit
Steel Chemical Energy, 0.6%-C (LHV)	277,546	kW
Energy Input	**Value**	**Unit**
Methane Chemical Energy (LHV)	39,179	kW
Carbon Chemical Energy (LHV)	40,992	kW
Hydrogen Chemical Energy (LHV)	296,137	kW
Process Gas Recycle	1,176	kW
H_2 Heater Air Blower	52	kW
Scrubber Water Circulation Pump	153	kW
Cooling Tower Fans	215	kW
Cooling Tower Water Circulation Pump	931	kW
Oxygen PSA	10,726	kW
EAF Reactor	47,820	kW
EAF Induced Draft Fan	65	kW
Ladle Refining	3,657	kW
Miscellaneous Balance of Plant	8,236	kW
Energy Efficiency	**Value**	**Unit**
Steel Reduction Thermal Efficiency	61.77	%

Table S8: Steel Plant Economics for the H_2-DRI-B Case

Overnight Cost	Value	Unit
Total Plant Cost	633,032	$ (thousands)
Preproduction Cost	87,019	$ (thousands)
Inventory Capital Cost	46,047	$ (thousands)
Initial Catalyst, Sorbent & Chemicals Cost	0	$ (thousands)
Land	900	$ (thousands)
Other Owners' Costs (18.4% of TPC)	94,955	$ (thousands)
Financing Costs	17,092	$ (thousands)
Fixed Operating Cost	**Value**	**Unit**
Annual Labor Cost	93,720	$ (thousands)
Annual Tax and Insurance Cost	12,661	$ (thousands)
Variable Operating Cost	**Value**	**Unit**
Annual Iron Ore Pellet Feedstock Cost	221,528	$ (thousands)
Annual Natural Gas Cost	10,455	$ (thousands)
Annual Hydrogen Cost	118,870	$ (thousands)
Annual Electricity Cost	53,777	$ (thousands)
Annual Maintenance Materials Cost	9,367	$ (thousands)
Annual Chemical, Catalyst & Disposal Costs	20,315	$ (thousands)
Economic Performance Metrics	**Value**	**Unit**
Specific Steel Plant Cost	532	$/metric tonne steel
1st Year Levelized Cost of Steel	582.18	$/metric tonne steel

S4. Performance summary H_2-DRI-T case

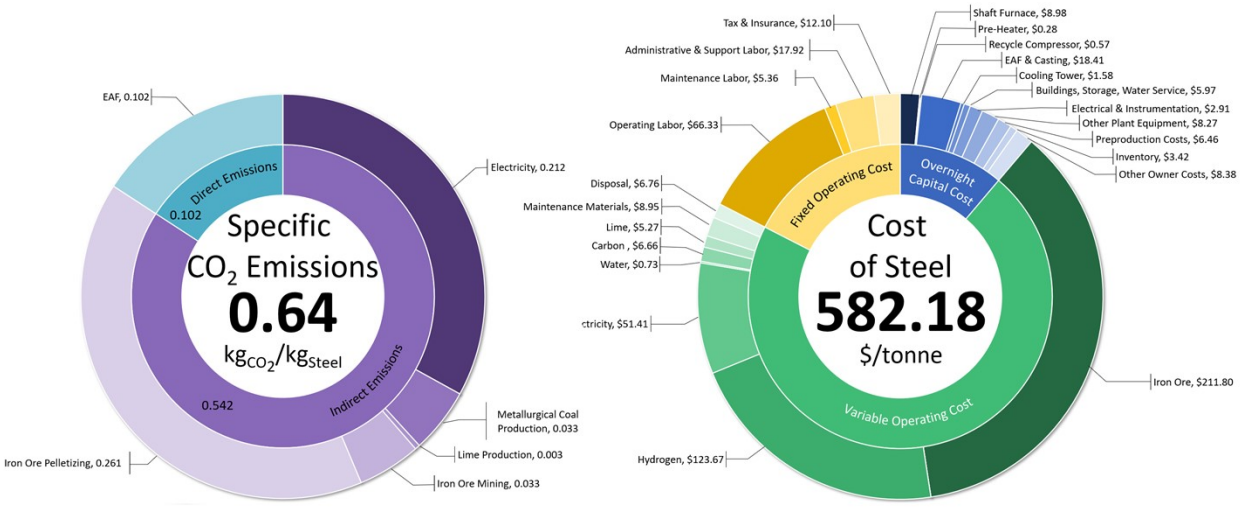

Figure S4: Breakdown of carbon dioxide emissions (left) and levelized cost of steel (right) for the H_2-DRI-T case.

Table S9: Steel Plant Performance for the H_2-DRI-T Case

Plant Design Capacity	Value	Unit
Steel Slab Production Capacity	1,162,120	metric tonnes/year
Plant Capacity Factor	90	%
Actual Steel Slab Production	1,045,908	metric tonnes/year
Consumables at 90% CF	**Value**	**Unit**
Iron Ore Pellets	1,704,063	metric tonnes/year
Hydrogen Gas	79,466	metric tonnes/year
Natural Gas	0	GJ/year
Electricity	575,705	MWh/year
Carbon	35,511	metric tonnes/year
Lime	53,537	metric tonnes/year
Raw Water Withdrawal	1,255,384	metric tonnes/year
Emissions at 90% CF	**Value**	**Unit**
Direct Carbon Dioxide Emissions	106,514	metric tonnes/year
Specific Direct CO_2 Emission	0.102	kg_{CO2}/kg_{Steel}
Specific Indirect CO_2 Emission	0.542 (0.576)*	kg_{CO2}/kg_{Steel}
Slag	182,335	metric tonnes/year
Surface Water Discharge	457,644	metric tonnes/year

*Considering an emission factor of 0.45 kg_{CO2}/kg_{H2}

Table S10: Steel Plant Energy Balance for the H_2-DRI-T Case at Full Capacity

Energy Output	Value	Unit
Steel Chemical Energy, 0.6%-C (LHV)	277,546	kW
Energy Input	**Value**	**Unit**
Methane Chemical Energy (LHV)	0	kW
Carbon Chemical Energy (LHV)	40,992	kW
Hydrogen Chemical Energy (LHV)	335,978	kW
Process Gas Recycle	1,176	kW
H_2 Heater Air Blower	47	kW
Scrubber Water Circulation Pump	153	kW
Cooling Tower Fans	214	kW
Cooling Tower Water Circulation Pump	929	kW
Oxygen PSA	10,726	kW
EAF Reactor	47,820	kW
EAF Induced Draft Fan	65	kW
Ladle Refining	3,657	kW
Miscellaneous Balance of Plant	8,236	kW
Energy Efficiency	**Value**	**Unit**
Steel Reduction Thermal Efficiency	61.68	%

Table S11: Steel Plant Economics for the H_2-DRI-T Case

Overnight Cost	Value	Unit
Total Plant Cost	632,923	$ (thousands)
Preproduction Cost	87,017	$ (thousands)
Inventory Capital Cost	46,046	$ (thousands)
Initial Catalyst, Sorbent & Chemicals Cost	0	$ (thousands)
Land	900	$ (thousands)
Other Owners' Costs (18.4% of TPC)	94,938	$ (thousands)
Financing Costs	17,089	$ (thousands)
Fixed Operating Cost	**Value**	**Unit**
Annual Labor Cost	93,719	$ (thousands)
Annual Tax and Insurance Cost	12,658	$ (thousands)
Variable Operating Cost	**Value**	**Unit**
Annual Iron Ore Pellet Feedstock Cost	221,528	$ (thousands)
Annual Natural Gas Cost	0	$ (thousands)
Annual Hydrogen Cost	129,349	$ (thousands)
Annual Electricity Cost	53,771	$ (thousands)
Annual Maintenance Materials Cost	9,365	$ (thousands)
Annual Chemical, Catalyst & Disposal Costs	20,312	$ (thousands)
Economic Performance Metrics	**Value**	**Unit**
Specific Steel Plant Cost	532	$/metric tonne steel
1st Year Levelized Cost of Steel	582.18	$/metric tonne steel

S5. Sensitivity of the break-even cost of hydrogen to changes in natural gas and electricity prices

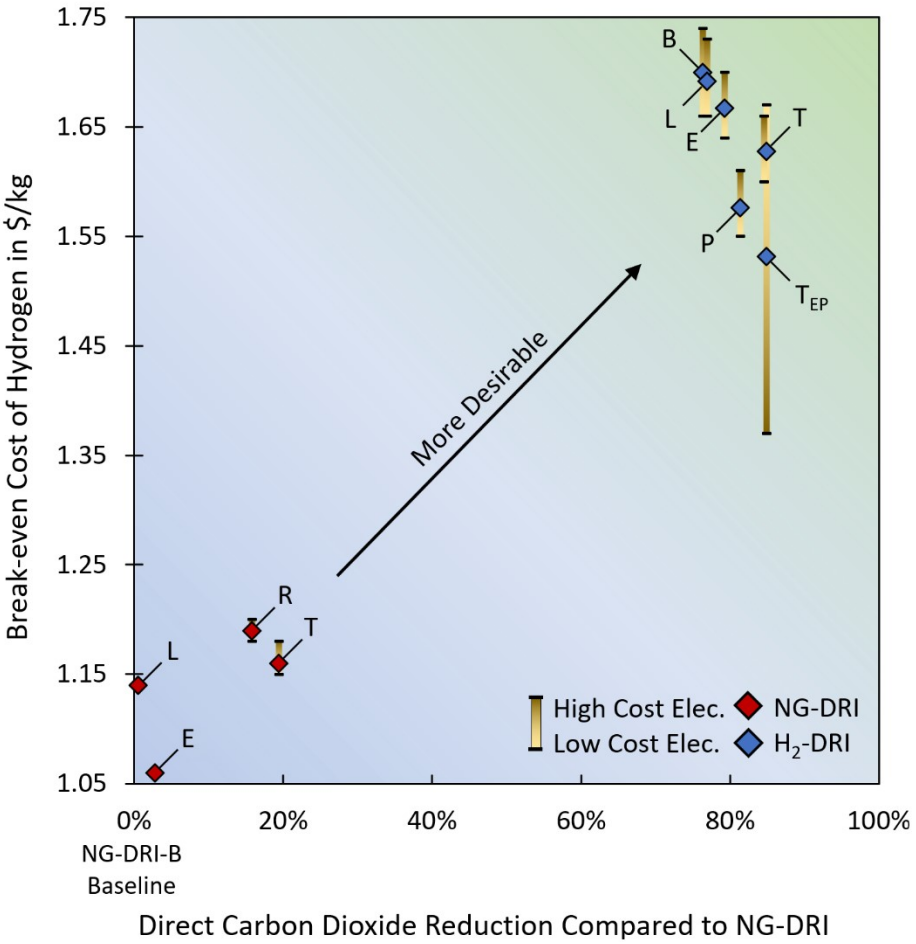

Figure S5: Direct carbon dioxide emission reduction potential and associated H_2 break-even prices for the various NG consuming processes in an integrated DRI steel mill. The results of the electricity price sensitivities are indicated by the yellow bars for a range of $180.00/MWh (dark yellow, representative for Massachusetts, Rhode Island and Alaska) to $20.00/MWh (light yellow, representative of future renewable electricity prices, lowest electricity prices in the US can be found in Louisiana and Texas at ~$55.00/MWh).

Table S12: Sensitivity Analysis of NG Price and Electricity Price and their Impact upon the Break-even LCOH

Scenario	NG-DRI-B	NG-DRI-R	NG-DRI-E	NG-DRI-L	NG-DRI-T	H_2-DRI-B	H_2-DRI-P	H_2-DRI-E	H_2-DRI-L	H_2-DRI-T	H_2-DRI-T_{EP}
Emission Reduction	Reference	2.8%	0.6%	15.9%	19.4%	76.3%	79.3%	76.9%	81.3%	84.9%	84.9%
	LSPC ($/t)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)	LCOH ($/kg)
Base Case	582.18	1.06	1.14	1.19	1.16	1.70	1.67	1.69	1.58	1.63	1.53
NG ($63.69/MWh)	665.50	1.92	2.07	2.14	2.10	2.82	2.78	2.81	2.62	2.72	2.71
NG ($8.85/MWh)	505.66	0.27	0.29	0.31	0.30	0.67	0.65	0.66	0.62	0.62	0.46
Electricity ($180.00/MWh)	632.49	1.06	1.14	1.20	1.18	1.74	1.70	1.73	1.61	1.66	1.37
Electricity ($20.00/MWh)	539.54	1.06	1.14	1.18	1.15	1.66	1.64	1.66	1.55	1.60	1.67

References

1. Kirschen, M., Pfeifer, H., Wahlers, F.-J. & Mees, H. OFF-GAS MEASUREMENTS FOR MASS AND ENERGY BALANCESOF A STAINLESS STEEL EAF. *59th Electr. Furn. Conf. Phoenix USA* (2001).

2. Gandt, K., Meier, T., Echterhof, T. & Pfeifer, H. Heat recovery from EAF off-gas for steam generation: analytical exergy study of a sample EAF batch. *Ironmak. Steelmak.* (2016) doi:10.1080/03019233.2016.1155812.