

Supplementary Material file for the article:

Sustainability Analysis of Methane-to-Hydrogen-to-Ammonia Conversion by Integration of High-Temperature Plasma and Non-Thermal Plasma Processes

Jose Osorio-Tejada^{1,7,*}, Kevin van 't Veer³, Nguyen Van Duc Long^{1,2}, Nam N. Tran^{2,4}, Laurent Fulcheri⁵, Bhaskar Patil⁶, Annemie Bogaerts³, Volker Hessel^{1,2}

¹School of Engineering, University of Warwick, United Kingdom

²School of Chemical Engineering and Advanced Materials, University of Adelaide, Australia

³Department of Chemistry, Research Group PLASMANT, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium

⁴Department of Chemical Engineering, Can Tho University, Vietnam

⁵MINES ParisTech, PSL-Research University, PERSEE, Sophia-Antipolis, France

⁶Nouryon, Capability Group, Process Technology - Reaction Engineering, Deventer/the Netherlands

⁷Territorial Environmental Management Research Group -GAT-, Universidad Tecnológica de Pereira, Pereira, Colombia

* Authors for correspondence: jose.osorio-tejada@warwick.ac.uk

This Supplementary Material file presents the results of the techno-economic analyses for each ammonia production pathway in which capital and operating costs and the unitary cost of ammonia production are detailed. The methods, references, and assumptions for the calculation process are described in the main article.

Contents

- Table S1.** Capital costs for the stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S2.** Operating costs for the stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S3.** Total annual costs for the stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh
- Table S4.** Unitary cost of production for the Stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S5.** Capital costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S6.** Operating costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S7.** Total annual costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh
- Table S8.** Unitary cost of production for the non-integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh
- Table S9.** Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 1.09 g NH₃/kWh
- Table S10.** Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 1.09 g NH₃/kWh
- Table S11.** Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 1.09 g NH₃/kWh
- Table S12.** Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 1.09 g NH₃/kWh
- Table S13.** Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh
- Table S14.** Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh
- Table S15.** Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh
- Table S16.** Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh
- Table S17.** Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 900 g NH₃/kWh
- Table S18.** Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 900 g NH₃/kWh
- Table S19.** Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 900 g NH₃/kWh
- Table S20.** Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 900 g NH₃/kWh
- Table S21.** Capital costs for the conventional SMR-HB plant (106,000 t NH₃/year).
- Table S22.** Operating costs for the conventional SMR-HB plant (106,000 t NH₃/year).
- Table S23.** Total annual costs for the conventional SMR-HB plant (106,000 t NH₃/year).
- Table S24.** Unitary cost of production for the conventional SMR-HB plant (106,000 t NH₃/year)
- Table S25.** Capital costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh
- Table S26.** Operating costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh
- Table S27.** Total annual costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh
- Table S28.** Unitary cost of production for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh

Table S1

Capital costs for the Stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
	377,201,62	
Purchase Cost of Equipment (PCE)	1	100%
Heat exchangers	1,018,542	0.3%
Columns and vessels	1,371,528	0.4%
NTP reactor	311,076,248	82.5%
PSA unit	2,369,389	0.6%
PEM electrolyser	61,365,913	16.3%
	645,014,77	
Direct costs	1	Direct cost factors
Purchase Cost of Equipment (PCE)	377,201,621	100% of PCE
Equipment installation	94,300,405	25% of PCE
Instrumentation/controls installation	22,632,097	6% of PCE
Piping installation	37,720,162	10% of PCE
Electrical systems installation	37,720,162	10% of PCE
Buildings	37,720,162	10% of PCE
Site development	37,720,162	10% of PCE
	308,588,64	
Indirect costs	6	Indirect cost factors
Engineering and supervision	32,250,739	5% of direct costs
Construction expenses	38,700,886	6% of direct costs
Contractor fees	79,212,340	21% of PCE
Contingency fees	158,424,681	42% of PCE
	953,603,41	
Fixed Capital Investment (FCI)	7	Direct costs + Indirect costs
Working Capital Investment (WCI)	168,282,956	15% of TCI
Total Capital Investment (TCI)	1,121,886,373	WCI + FCI

Table S2

Operating costs for the Stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh

OPERATING COSTS	Annual costs (US \$2020)	
	3,357,	
Raw materials	492	
Deionised Water	1,435,65	
Catalysts	1,921,84	Electrolyser
	1	NTP reactor (1.39 g Fe/kg NH ₃)
Utilities	6,687,566,420	
Electricity for Electrolyser	53,239,81	
Electricity for PSA unit	9	
Electricity for NTP	498,2	
Heat	91	
	6,632,261,00	
	0	
	1,567,31	
	0	
Total variable costs	6,690,923,9	Raw materials + Utilities
	50,787,	
Total fixed costs	378	
Maintenance	19,072,06	
Operating labour	8	2% of FCI
	800,0	Actuals (\$)

	00	
	7,948,82	
Plan overheads	7	5% of total operating costs
	80,0	
Laboratory charges	00	10% of operating labour
	3,814,41	
Insurance	4	0.4% of FCI
	19,072,06	
Taxes and royalties	8	2% of FCI
	749,079,03	
General expenses	2	10% of total operating costs
Total Operating costs	7,490,790,3	Variable costs + Fixed Costs + General expenses
	22	

Table S3

Total annual costs for the Stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh

	Electrolysis		PSA section		NTP section		TOTAL (US\$)
section							
Annualised capital costs*	20,3		78		104,1		125,3
	96,732		7,535		89,576		73,843
Capital costs	155,1		5,99		792,4		
	39,164		0,053		74,200		
Electrolyser	61,36		2,369		Reactor and	313,46	
	5,913	PSA unit	,389		aux.	6,319	
Installation	93,77	Installation	3,620		Installation	479,00	
	3,251		,664			7,882	
Operating costs	69,233,09		87		7,420,6		7,490,7
	0		3,084		84,149		90,322
Process Water	1,43				Catalyst	1,92	
	5,652					1,841	
Electricity	53,23	Electricity	498,		Electricity	6,632,26	
	9,819		291			1,000	
					Heat	1,56	
						7,310	
Fixed & general	14,557,619	Fixed & general	374,793		Fixed & general	784,93	
						3,998	
TOTAL	89,6		1,66		7,524,8		7,616,1
	31,296		0,632		72,237		64,165

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S4

Unitary cost of production for the Stand-alone (electrolyser-NTP) plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh

Section (cost type)		Unitary cost of production (US\$/t NH ₃)
Electrolysis section	H ₂ production (capex)	192

	H ₂ production (opex)	653
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	8
NTP section	NH ₃ synthesis (capex)	983
	NH ₃ synthesis (opex)	70,006
TOTAL		71,851

Table S5

Capital costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	386,429,738	100%
Heat exchangers	1,018,542	0.3%
Methanator	10,296,599	2.7%
NTP Reactor	311,076,248	80.5%
Columns and vessels	1,371,528	0.4%
PSA unit	2,369,389	0.6%
HTP reactors	60,297,431	15.6%
	660,794,85	
Direct costs	1	Direct cost factors
Purchase Cost of Equipment (PCE)	386,429,738	100% of PCE
Equipment installation	96,607,434	25% of PCE
Instrumentation/controls installation	23,185,784	6% of PCE
Piping installation	38,642,974	10% of PCE
Electrical systems installation	38,642,974	10% of PCE
Buildings	38,642,974	10% of PCE
Site development	38,642,974	10% of PCE
	316,138,16	Indirect cost factors
Indirect costs	8	
Engineering and supervision	33,039,743	5% of direct costs
Construction expenses	39,647,691	6% of direct costs
Contractor fees	81,150,245	21% of PCE
Contingency fees	162,300,490	42% of PCE
Fixed Capital Investment (FCI)	976,933,020	Direct costs + Indirect costs
Working Capital Investment (WCI)	172,399,945	15% of TCI
Total Capital Investment (TCI)	1,149,332,964	WCI + FCI

Table S6

Operating costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 0.8 g NH₃/kWh

OPERATING COSTS	Annual costs (US \$2020)	
Raw materials	18,532,757	
Natural gas	16,334,049	HTP reactors
Nickel	276,896	Methanator (0.0033 g Ni/kg NH ₃)
	1,921,84	NTP reactor (1.39 g Fe/kg NH ₃)
Catalysts	1	
Utilities	6,660,794,329	
Electricity for HTP	26,467,728	
Electricity for PSA unit	498,291	
Electricity for NTP	6,632,261,000	
Heat	1,567,31	
	0	
Total variable costs	6,679,327,086	Raw materials + Utilities
	52,000,	
Total fixed costs	517	
Maintenance	19,538,660	2% of FCI
	800,0	
Operating labour	00	Actuals (\$)
Plan overheads	8,135,464	5% of total operating costs
	80,0	
Laboratory charges	00	10% of operating labour
Insurance	3,907,732	0.4% of FCI
Taxes and royalties	19,538,660	2% of FCI
	747,925,28	
General expenses	9	10% of total operating costs
	7,490,790,3	Variable costs + Fixed Costs +
Total Operating costs	22	
		General expenses
Credits	58,210,308	Carbon black co-product
Total Operating costs (-credits)	7,421,042,585	Total operating cost - credits

Table S7

Total annual costs for the non-integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh

section	HTP	PSA section	NTP section	TOTAL (US\$)
Annualised capital costs*	23,4 63,963	78 7,535	104,1 89,576	128,4 41,074
Capital costs	178,4 68,766	5,99 0,053	792,4 74,200	
HTP reactors	70,594,02 9	PSA unit 2,369 ,389	Reactor and aux. 313,46 6,319	
Installation	107,874,7 36	Installation 3,620 ,664	Installation 479,00 7,882	
Operating costs	57,4 02,052	87 2,928	7,420,9 77,913	7,479,2 52,893
Methane	16,334,04 9		Catalyst 1,92 1,812	
Electricity	26,467,728	Electricity 498, 291	Electricity 6,632,26 1,000	
Nickel catalyst	276,896		Heat 1,56 7,310	

Fixed & general	14,323,379	Fixed & general	374,637	Fixed & general	785,227,790
Carbon black credits	-				
	58,210,308				
TOTAL	22,655,707	1,660,463		7,525,167,489	7,549,483,659

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S8

Unitary cost of production for the non-integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 0.8 g NH₃/kWh

Section (cost type)		Unitary cost of production (US\$/t NH ₃)
HTP section	H ₂ production (capex)	221
	H ₂ production (opex)	542
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	8
NTP section	NH ₃ synthesis (capex)	983
	NH ₃ synthesis (opex)	70,009
Credits	Carbon black	-549
TOTAL		71,222

Table S9

Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 1.09 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	333,798,611	100%
Heat exchangers	1,018,542	0.3%
Methanator	10,296,599	3.1%
NTP Reactor	258,445,122	77.4%
Columns and vessels	1,371,528	0.4%
PSA unit	2,369,389	0.7%
HTP reactors	60,297,431	18.1%
Direct costs	570,795,62	Direct cost factors

5		
Purchase Cost of Equipment (PCE)	333,798,611	100% of PCE
Equipment installation	83,449,653	25% of PCE
Instrumentation/controls installation	20,027,917	6% of PCE
Piping installation	33,379,861	10% of PCE
Electrical systems installation	33,379,861	10% of PCE
Buildings	33,379,861	10% of PCE
Site development	33,379,861	10% of PCE
Indirect costs	273,080,644	Indirect cost factors
Engineering and supervision	28,539,781	5% of direct costs
Construction expenses	34,247,738	6% of direct costs
Contractor fees	70,097,708	21% of PCE
Contingency fees	140,195,417	42% of PCE
Fixed Capital Investment (FCI)	843,876,269	Direct costs + Indirect costs
Working Capital Investment (WCI)	148,919,342	15% of TCI
Total Capital Investment (TCI)	992,795,610	WCI + FCI

Table S10

Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 1.09 g NH₃/kWh

OPERATING COSTS	Annual costs (US \$2020)	
Raw materials	18,532,757	
Natural gas	16,334,049	HTP reactors
Nickel	276,896	Methanator (0.0033 g Ni/kg NH ₃)
	1,921,84	
Catalysts	1	NTP reactor (1.39 g Fe/kg NH ₃)
Utilities	4,896,612,340	
Electricity for HTP	26,467,728	
Electricity for PSA unit	498,291	
Electricity for NTP	4,869,646,321	
Total variable costs	4,915,145,097	Raw materials + Utilities
	45,081,566	
Total fixed costs	566	
Maintenance	16,877,525	2% of FCI
	800,0	
Operating labour	00	Actuals (\$)
Plan overheads	7,071,010	5% of total operating costs
	80,0	
Laboratory charges	00	10% of operating labour
Insurance	3,375,505	0.4% of FCI
Taxes and royalties	16,877,525	2% of FCI
General expenses	551,136,296	10% of total operating costs
Total Operating costs	5,511,362,959	Variable costs + Fixed Costs + General expenses
Credits	58,210,308	Carbon black co-product
Total Operating costs (-credits)	5,453,152,651	Total operating cost - credits

Table S11

Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 1.09 g NH₃/kWh

	HTP section	PSA section	NTP section	TOTAL (US\$)
--	--------------------	--------------------	--------------------	---------------------

Annualised capital costs*	23,4 63,963		78 7,535		86,696,1 03	110,9 47,600
Capital costs	178,4 68,766		5,99 0,053		659,4 17,449	
HTP reactors	70,594,02 9	PSA unit	2,369 ,389	Reactor and aux.	260,835,1 92	
Installation	107,874,7 36	Installation	3,620 ,664	Installation	398,582,2 57	
Operating costs	57,4 43,254		87 4,165		5,453,0 45,540	5,511,3 62,959
Methane	16,334,04 9			Catalyst	1,92 1,812	
Electricity	26,467,728	Electricity	498, 291	Electricity	4,869,64 6,321	
Nickel catalyst	276,896					
Fixed & general	14,364,5 81	Fixed & general	375,874	Fixed & general	581,477,4 07	
Carbon black credits	- 58,210,308					
TOTAL	22,696,9 09		1,661, 700		5,539,74 1,642	5,564,1 00,251

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S12

Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 1.09 g NH₃/kWh

Section (cost type)		Unitary cost of production (US\$/t NH₃)
HTP section	H ₂ production (capex)	221
	H ₂ production (opex)	542
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	8
NTP section	NH ₃ synthesis (capex)	818
	NH ₃ synthesis (opex)	51,444
Credits	Carbon black	-549
TOTAL		52,492

Table S13

Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	108,108,456	100%
Heat exchangers	1,018,542	0.9%
Methanator	10,296,599	9.5%
NTP Reactor	32,754,967	30.3%
Columns and vessels	1,371,528	1.3%
PSA unit	2,369,389	2.2%
HTP reactors	60,297,431	55.8%
Direct costs	184,865,460	Direct cost factors
Purchase Cost of Equipment (PCE)	108,108,456	100% of PCE
Equipment installation	27,027,114	25% of PCE
Instrumentation/controls installation	6,486,507	6% of PCE
Piping installation	10,810,846	10% of PCE
Electrical systems installation	10,810,846	10% of PCE
Buildings	10,810,846	10% of PCE
Site development	10,810,846	10% of PCE
Indirect costs	88,443,528	Indirect cost factors
Engineering and supervision	9,243,273	5% of direct costs
Construction expenses	11,091,928	6% of direct costs
Contractor fees	22,702,776	21% of PCE
Contingency fees	45,405,552	42% of PCE
Fixed Capital Investment (FCI)	273,308,988	Direct costs + Indirect costs
Working Capital Investment (WCI)	48,230,998	15% of TCI
Total Capital Investment (TCI)	321,539,986	WCI + FCI

Table S14

Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh

OPERATING COSTS	Annual costs (US \$2020)	
Raw materials	18,532,757	
Natural gas	16,334,049	HTP reactors
Nickel	276,896	Methanator (0.0033 g Ni/kg NH ₃)
Catalysts	1,921,841	NTP reactor (1.39 g Fe/kg NH ₃)
Utilities	182,686,402	
Electricity for HTP	26,467,728	
Electricity for PSA unit	498,291	
Electricity for NTP	155,720,384	
Total variable costs	201,219,160	Raw materials + Utilities
Total fixed costs	15,412,067	
Maintenance	5,466,180	2% of FCI
	800,0	
Operating labour	00	Actuals (\$)
Plan overheads	2,506,472	5% of total operating costs
	80,0	
Laboratory charges	00	10% of operating labour
Insurance	1,093,236	0.4% of FCI
Taxes and royalties	5,466,180	2% of FCI
General expenses	24,070,136	10% of total operating costs
Total Operating costs	240,701,363	Variable costs + Fixed Costs + General expenses
Credits	58,210,308	Carbon black co-product
Total Operating costs (-credits)	182,491,056	Total operating cost - credits

Table S15

Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh

	HTP section	PSA section	NTP section	TOTAL (US\$)
Annualised capital costs*	23,4 63,963	78 7,535	11,681,4 67	35,93 2,965
Capital costs	178,4 68,766	5,99 0,053	88,850,1 69	
HTP reactors	70,594,029	PSA unit 2,369,389	Reactor and aux. 35,145,037	
Installation	107,874,736	Installation 3,620,664	Installation 53,705,132	
Operating costs	58,2 95,776	895,68 0	181,509 ,908	240,701 ,363
Methane	16,334,049		Catalyst 1,921,812	
Electricity	26,467,728	Electricity 498,291	Electricity 155,720,384	
Nickel catalyst	276,896			
Fixed & general	15,217,102	Fixed & general 397,389	Fixed & general 23,867,712	
Carbon black credits	- 58,210,308			
TOTAL	23,549,4 31	1,683, 215	193,191, 375	218,424 ,021

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S16

Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh

Section (cost type)		Unitary cost of production (US\$/t NH ₃)
HTP section	H ₂ production (capex)	221
	H ₂ production (opex)	550
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	8
NTP section	NH ₃ synthesis (capex)	110
	NH ₃ synthesis (opex)	1,712
Credits	Carbon black	-549

TOTAL	2,061
--------------	--------------

Table S17

Capital costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 900 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	82,787,499	100%
Heat exchangers	1,018,542	1.2%
Methanator	10,296,599	12.4%
NTP Reactor	7,434,010	9.0%
Columns and vessels	1,371,528	1.7%
PSA unit	2,369,389	2.9%
HTP reactors	60,297,431	72.8%
Direct costs	141,566,624	Direct cost factors
Purchase Cost of Equipment (PCE)	82,787,499	100% of PCE
Equipment installation	20,696,875	25% of PCE
Instrumentation/controls installation	4,967,250	6% of PCE
Piping installation	8,278,750	10% of PCE
Electrical systems installation	8,278,750	10% of PCE
Buildings	8,278,750	10% of PCE
Site development	8,278,750	10% of PCE
Indirect costs	67,728,453	Indirect cost factors
Engineering and supervision	7,078,331	5% of direct costs
Construction expenses	8,493,997	6% of direct costs
Contractor fees	17,385,375	21% of PCE
Contingency fees	34,770,750	42% of PCE
Fixed Capital Investment (FCI)	209,295,077	Direct costs + Indirect costs
Working Capital Investment (WCI)	36,934,425	15% of TCI
Total Capital Investment (TCI)	246,229,502	WCI + FCI

Table S18

Operating costs for the integrated HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 900 g NH₃/kWh

OPERATING COSTS	Annual costs (US \$2020)	
Raw materials	18,532,757	
Natural gas	16,334,049	HTP reactors
Nickel	276,896	Methanator (0.0033 g Ni/kg NH ₃)
Catalysts	1,921,841	NTP reactor (1.39 g Fe/kg NH ₃)
Utilities	40,115,908	
Electricity for HTP	26,467,728	
Electricity for PSA unit	498,291	
Electricity for NTP	13,149,889	
Total variable costs	58,648,665	Raw materials + Utilities
Total fixed costs	12,083,344	

Maintenance	4,185,902 800,0	2% of FCI
Operating labour	00	Actuals (\$)
Plan overheads	1,994,361 80,0	5% of total operating costs
Laboratory charges	00	10% of operating labour
Insurance	837,180	0.4% of FCI
Taxes and royalties	4,185,902	2% of FCI
General expenses	7,859,112	10% of total operating costs
Total Operating costs	78,591,121	Variable costs + Fixed Costs + General expenses
Credits	58,210,308	Carbon black co-product
Total Operating costs (-credits)	20,380,813	Total operating cost - credits

Table S19

Total annual costs for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 900 g NH₃/kWh

	HTP section	PSA section	NTP section	TOTAL (US\$)
Annualised capital costs*	23,4 63,963	78 7,535	3,265,31 7	27,516,8 14
Capital costs	178,4 68,766	5,99 0,053	24,836,2 58	
HTP reactors	70,594,02 9	PSA unit 2,369 ,389	Reactor and aux. 9,824,080	
Installation	107,874,7 36	Installation 3,620 ,664	Installation 15,012,17 7	
Operating costs	59,1 54,988	910,89 0	18,525, 243	78,591, 121
Methane	16,334,04 9		Catalyst 1,92 1,812	
Electricity	26,467,728	Electricity 498, 291	Electricity 13,149,88 9	
Nickel catalyst	276,896			
Fixed & general	16,076,3 15	Fixed & general 412,600	Fixed & general 3,453,542	
Carbon black credits	- 58,210,308			
TOTAL	24,408,6 43	1,698, 425	21,790,5 59	47,897, 627

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S20

Unitary cost of production for the integrated HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 900 g NH₃/kWh

Section (cost type)	Unitary cost of production
---------------------	-------------------------------

		(US\$/t NH ₃)
HTP section	H ₂ production (capex)	221
	H ₂ production (opex)	558
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	9
NTP section	NH ₃ synthesis (capex)	31
	NH ₃ synthesis (opex)	175
Credits	Carbon black	-549
TOTAL		452

Table S21

Capital costs for the conventional SMR-HB plant (106,000 t NH₃/year).

CAPITAL COSTS*	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	31,925,974	100%
Heat exchangers	1,309,406	4.1%
Columns and vessels	2,686,506	8.4%
Reactors	1,497,849	4.7%
Compressors and expanders	26,318,385	82.4%
Membrane	113,829	0.4%
Direct costs	108,548,312	Direct cost factors
Purchase Cost of Equipment (PCE)	31,925,974	100% of PCE
Equipment installation	15,005,208	47% of PCE
Instrumentation/controls installation	5,746,675	18% of PCE
Piping installation	21,071,143	66% of PCE
Electrical systems installation	3,511,857	11% of PCE
Buildings	5,746,675	18% of PCE
Site development	3,192,597	10% of PCE
Utilities/services	22,348,182	70% of PCE
Indirect costs	43,738,585	Indirect cost factors
Engineering and supervision	10,535,571	33% of direct costs
Construction expenses	13,089,649	41% of direct costs
Contractor fees	6,704,455	21% of PCE
Contingency fees	13,408,909	42% of PCE
Fixed Capital Investment (FCI)	152,286,897	Direct costs + Indirect costs
Working Capital Investment (WCI)	26,874,158	15% of TCI
Total Capital Investment (TCI)	179,161,055	WCI + FCI

Table S22

Operating costs for the conventional SMR-HB plant (106,000 t NH₃/year).

OPERATING COSTS	Annual costs (US \$2020)	
Raw materials	10,459,182	Consumption per kg NH₃
Natural gas	7,771,717	0.01833 MMBTU
Cobalt molybdenum	621,305	0.00133 g
Zinc oxide	254,776	0.01961 g
Nickel 1	692,333	0.00833 g
Nickel 2	553,977	0.00667 g
Chromium oxide	91,195	0.01039 g
Copper oxide	40,817	0.03098 g
Nickel 3	276,896	0.00333 g
Iron	98,319	0.05294 g
Process Water	57,846	0.00831 m ³
Utilities	17,071,849	
Cooling	4,459,986	0.68 m ³
Electricity	2,720,822	0.513 kWh
Steam	3,559,683	1.84 kg
Heat	6,331,358	0.018 GJ
Total variable costs	27,531,041	Raw materials + Utilities
Total fixed costs	19,383,559	
Maintenance	7,614,345	5% of FCI
	1,400,000	
Operating labour	280,000	Actuals (\$)
Supervision	3,717,738	20% of operating labour
Plant overheads	280,000	7% of total operating costs
Laboratory charges	000	20% of operating labour
Operating supplies	1,522,869	1% of FCI
Insurance	1,522,869	1% of FCI
Taxes and royalties	3,045,738	2% of FCI

General expenses	5,212,732	10% of total operating costs
Total Operating costs	52,127,380	Variable costs + Fixed Costs + General expenses
Credits 1	9,098,960	Steam by-products
Credits 2	1,145,083	Hydrogen by-products
Total Operating costs (-credits)	41,883,279	Total operating cost - credits

Table S23

Total annual costs for the conventional SMR-HB plant (106,000 t NH₃/year).

	SMR-HB costs	TOTAL (US\$)
Annualised capital costs*	20,0 21,733	20,021,7 33
Capital costs	152,2 86,897	
Equipment costs	31,925,97 4	
Installation	120,360,9 23	
Operating costs	52,127,32 2	52,127, 322
Materials	10,459,18 2	
Utilities	17,071,84 9	
Fixed & general	24,596,29 1	
Steam & H ₂ credits	- 10,244,043	
TOTAL	61,905,01 2	61,905, 012

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S24

Unitary cost of production for the conventional SMR-HB plant (106,000 t NH₃/year)

Section (cost type)		Unitary cost of production (US\$/t NH ₃)
SMR-	NH ₃ production (capex)	189
HB	NH ₃ production (opex)	492
Credits	Steam and H ₂ by-products	-97
TOTAL		584

Table S25

Capital costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh

CAPITAL COSTS	(US \$2020)	(%)
Purchase Cost of Equipment (PCE)	114,553,900	100%
Heat exchangers	1,018,542	1%
Membrane separator	16,742,043	15%
NTP Reactor	32,754,967	29%
Columns and vessels	1,371,528	1%
PSA unit	2,369,389	2%
HTP reactors	60,297,431	53%
Direct costs	195,887,170	Direct cost factors
Purchase Cost of Equipment (PCE)	114,553,900	100% of PCE
Equipment installation	28,638,475	25% of PCE
Instrumentation/controls installation	6,873,234	6% of PCE
Piping installation	11,455,390	10% of PCE
Electrical systems installation	11,455,390	10% of PCE
Buildings	11,455,390	10% of PCE
Site development	11,455,390	10% of PCE
Indirect costs	93,716,546	Indirect cost factors
Engineering and supervision	9,794,358	5% of direct costs
Construction expenses	11,753,230	6% of direct costs
Contractor fees	24,056,319	21% of PCE
Contingency fees	48,112,638	42% of PCE
Fixed Capital Investment (FCI)	289,603,716	Direct costs + Indirect costs

Working Capital Investment (WCI)	51,106,538	15% of TCI
Total Capital Investment (TCI)	340,710,254	WCI + FCI

Table S26

Operating costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year). NTP energy yield: 35.7 g NH₃/kWh

OPERATING COSTS		Annual costs (US \$2020)
Raw materials		18,255,861
Natural gas	16,334,049	HTP reactors
Catalysts	1,921,841	NTP reactor (1.39 g Fe/kg NH ₃)
Utilities		184,455,912
Electricity for HTP	28,237,238	
Electricity for PSA unit	498,291	
Electricity for NTP	155,720,384	
Total variable costs	202,711,773	Raw materials + Utilities
Total fixed costs		16,259,393
Maintenance	5,792,074	2% of FCI
	800,000	
Operating labour	00	Actuals (\$)
Plan overheads	2,636,830	5% of total operating costs
	80,000	
Laboratory charges	00	10% of operating labour
Insurance	1,158,415	0.4% of FCI
Taxes and royalties	5,792,074	2% of FCI
General expenses	24,330,130	10% of total operating costs
Total Operating costs	243,301,296	Variable costs + Fixed Costs + General expenses
Credits	58,210,308	Carbon black co-product
Total Operating costs (-credits)	185,090,988	Total operating cost - credits

Table S27

Total annual costs for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh

	HTP section	PSA section	NTP section	TOTAL (US\$)
Annualised capital costs*	25,606,292	78	11,681,467	38,075,294
Capital costs	194,763,493	5,990,053	88,850,169	
HTP reactors	77,039,474	PSA unit	2,369,389	Reactor and aux.
Installation	117,724,020	Installation	3,620,664	53,705,132
Operating costs	60,855,600	894,400	181,551,295	243,301,296
Methane	16,334,049			Catalyst
Electricity	28,237,238	Electricity	498,291	1,921,812
				Electricity
				155,720,384

Fixed & general	16,284,314	Fixed & general	396,110	Fixed & general	23,909,099
Carbon black credits	-				
	58,210,308				
TOTAL	86,461,892	1,681,935		193,232,762	223,166,282

* Only the Fixed Capital Investment (FCI) is annualised because the Working Capital Investment (WCI) is recovered at the end of the project.

Table S28

Unitary cost of production for the integrated (pre-separation) HTP-NTP plant (106,000 t NH₃/year) by sections. NTP energy yield: 35.7 g NH₃/kWh

Section (cost type)		Unitary cost of production (US\$/t NH ₃)
HTP section	H ₂ production (capex)	242
	H ₂ production (opex)	574
PSA section	N ₂ production (capex)	7
	N ₂ production (opex)	8
NTP section	NH ₃ synthesis (capex)	110
	NH ₃ synthesis (opex)	1,713
Credits	Carbon black	-549
TOTAL		2,105