

## Supplemental Information

### Nurturing the Blossoming Hydrogen Economy Using HBAT: Modelling Every Link in the H<sub>2</sub> Supply Chain

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## I. Economic constants and assumptions

HBAT's algorithm has many layers of calculations operating in parallel to produce results. Most of the specific calculations can be seen by downloading the newest version of HBAT and checking the cell equations. Equations 1 through 39 are shown in the main text, but supplementary equations and constants are shown in the following section. Unless otherwise noted, fluid properties were calculated using default user parameters at the equivalent rate of 50,000 kg H<sub>2</sub>/day.

Table S1.

Constant	Value	Units	Equation
A <sub>1</sub>	0.2016	-	1
A <sub>2</sub>	1.9608	-	1
A <sub>3</sub>	10000	hr kg <sup>-1</sup>	1
A <sub>4</sub>	0.961	-	1
A <sub>5</sub>	19.916	-	1
B <sub>1</sub>	-1.3028 x 10 <sup>-12</sup>	K <sup>-3</sup> psi <sup>-1</sup>	3
B <sub>2</sub>	1.4 x 10 <sup>-13</sup>	K <sup>-3</sup>	3
B <sub>3</sub>	1.6873 x 10 <sup>-9</sup>	K <sup>-2</sup> psi <sup>-1</sup>	3
B <sub>4</sub>	-1 x 10 <sup>-10</sup>	K <sup>-2</sup>	3
B <sub>5</sub>	-8.1388 x 10 <sup>-7</sup>	K <sup>-1</sup> psi <sup>-1</sup>	3
B <sub>6</sub>	4 x 10 <sup>-8</sup>	K <sup>-1</sup>	3
B <sub>7</sub>	1.732 x 10 <sup>-4</sup>	psi <sup>-1</sup>	3
B <sub>8</sub>	1.0001	-	3
C <sub>1</sub>	63027	USD	4
C <sub>2</sub>	0.0697	in <sup>-1</sup>	4
C <sub>3</sub>	251.737	USD in <sup>-2</sup>	4
C <sub>4</sub>	60848.1	USD in <sup>-1</sup>	4
C <sub>5</sub>	303657	USD	4
P <sub>in</sub>	1000	psi	1, 3
P <sub>out</sub>	700	psi	1, 3
ρ <sub>rel</sub>	0.06897	-	1
T	298.15	K	1, 3
Re <sub>HCOOH</sub>	53375	-	6
Re <sub>CH<sub>3</sub>OH</sub>	56103	-	6
Re <sub>NH<sub>3</sub></sub>	168623	-	6
Re <sub>HCOOCH<sub>3</sub></sub>	176294	-	6
ε	4.6 x 10 <sup>-5</sup>	m	6
X <sub>mat</sub>	0.75	-	7
%R <sub>1</sub>	100	%	24
%R <sub>2</sub>	5	%	24, 27

Supplemental equations:

$$(S1) \quad \dot{W}_{compressor} = Z_{LM} \cdot \frac{\dot{M} \cdot R \cdot T}{36M_W \cdot \epsilon} \cdot \frac{\gamma}{\gamma - 1} \cdot \left[ \left( \frac{P_{in}}{P_0} \right)^{\frac{\gamma-1}{N \cdot \gamma}} - 1 \right]$$

$$(S2) \quad \dot{W}_{liquefier} = 19.4312 \cdot \dot{M}^{0.9} \cdot N^{0.1}$$

$$(S3) \quad \text{Break Even Emissions Recovery Time } (t_{leak} \text{ in hrs}) = t_{leak} \cdot \frac{GWP \cdot \dot{M}}{\dot{C}F_{net}}$$

$$(S4) \quad \text{Break Even Leak Rate} = \frac{1}{\frac{GWP \cdot \dot{M}}{\dot{C}F_{net}} + 1} \cdot 100\%$$

## II. Supply chain specification table

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Table S2.

Supply Chain #	Production	Storage	Transport	End Use
1	Biomass Gasification	Gas H2	Pipeline	Fertilizer
2	Biomass Gasification	Gas H2	Pipeline	FCEV vehicle filling
3	Biomass Gasification	Gas H2	Railcar	Fertilizer
4	Biomass Gasification	Gas H2	Railcar	FCEV vehicle filling
5	Biomass Gasification	Formic Acid	Pipeline	Fertilizer
6	Biomass Gasification	Formic Acid	Pipeline	FCEV vehicle filling
7	Biomass Gasification	Formic Acid	Railcar	Fertilizer
8	Biomass Gasification	Formic Acid	Railcar	FCEV vehicle filling
9	Biomass Gasification	Liquid H2	Truck	Fertilizer
10	Biomass Gasification	Liquid H2	Truck	FCEV vehicle filling
11	Biomass Gasification	Liquid H2	Railcar	Fertilizer
12	Biomass Gasification	Liquid H2	Railcar	FCEV vehicle filling
13	CO2 Electrolysis PV Coupled	Methyl Formate	Pipeline	Fertilizer
14	CO2 Electrolysis PV Coupled	Methyl Formate	Pipeline	FCEV vehicle filling
15	CO2 Electrolysis PV Coupled	Methyl Formate	Railcar	Fertilizer

16	CO2 Electrolysis PV Coupled	Methyl Formate	Railcar	FCEV vehicle filling
17	CO2 Electrolysis PV Coupled	Formic Acid	Pipeline	Fertilizer
18	CO2 Electrolysis PV Coupled	Formic Acid	Pipeline	FCEV vehicle filling
19	CO2 Electrolysis PV Coupled	Formic Acid	Railcar	Fertilizer
20	CO2 Electrolysis PV Coupled	Formic Acid	Railcar	FCEV vehicle filling
21	CO2 Electrolysis PV Coupled	Methanol	Pipeline	Fertilizer
22	CO2 Electrolysis PV Coupled	Methanol	Pipeline	FCEV vehicle filling
23	CO2 Electrolysis PV Coupled	Methanol	Railcar	Fertilizer
24	CO2 Electrolysis PV Coupled	Methanol	Railcar	FCEV vehicle filling
25	N2 Electrolysis PV Coupled	Ammonia	Pipeline	Fertilizer
26	N2 Electrolysis PV Coupled	Ammonia	Pipeline	FCEV vehicle filling
27	N2 Electrolysis PV Coupled	Ammonia	Railcar	Fertilizer
28	N2 Electrolysis PV Coupled	Ammonia	Railcar	FCEV vehicle filling
29	H2O electrolysis PV Coupled	Gas H2	Pipeline	Fertilizer
30	H2O electrolysis PV Coupled	Gas H2	Pipeline	FCEV vehicle filling
31	H2O electrolysis PV Coupled	Gas H2	Railcar	Fertilizer
32	H2O electrolysis PV Coupled	Gas H2	Railcar	FCEV vehicle filling
33	H2O electrolysis PV Coupled	Formic Acid	Pipeline	Fertilizer
34	H2O electrolysis PV Coupled	Formic Acid	Pipeline	FCEV vehicle filling
35	H2O electrolysis PV Coupled	Formic Acid	Railcar	Fertilizer
36	H2O electrolysis PV Coupled	Formic Acid	Railcar	FCEV vehicle filling
37	H2O electrolysis PV Coupled	Liquid H2	Truck	Fertilizer
38	H2O electrolysis PV Coupled	Liquid H2	Truck	FCEV vehicle filling
39	H2O electrolysis PV Coupled	Liquid H2	Railcar	Fertilizer
40	H2O electrolysis PV Coupled	Liquid H2	Railcar	FCEV vehicle filling
41	SMR	Gas H2	Pipeline	Fertilizer

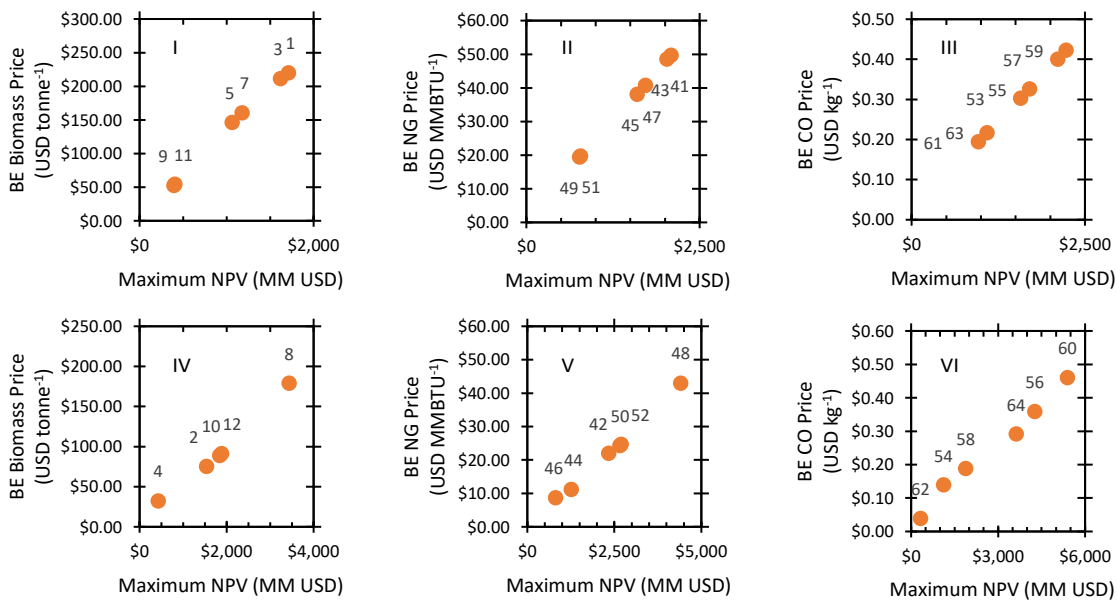
42	SMR	Gas H2	Pipeline	FCEV vehicle filling
43	SMR	Gas H2	Railcar	Fertilizer
44	SMR	Gas H2	Railcar	FCEV vehicle filling
45	SMR	Formic Acid	Pipeline	Fertilizer
46	SMR	Formic Acid	Pipeline	FCEV vehicle filling
47	SMR	Formic Acid	Railcar	Fertilizer
48	SMR	Formic Acid	Railcar	FCEV vehicle filling
49	SMR	Liquid H2	Truck	Fertilizer
50	SMR	Liquid H2	Truck	FCEV vehicle filling
51	SMR	Liquid H2	Railcar	Fertilizer
52	SMR	Liquid H2	Railcar	FCEV vehicle filling
53	CO Purchase	Methyl Formate	Pipeline	Fertilizer
54	CO Purchase	Methyl Formate	Pipeline	FCEV vehicle filling
55	CO Purchase	Methyl Formate	Railcar	Fertilizer
56	CO Purchase	Methyl Formate	Railcar	FCEV vehicle filling
57	CO Purchase	Formic Acid	Pipeline	Fertilizer
58	CO Purchase	Formic Acid	Pipeline	FCEV vehicle filling
59	CO Purchase	Formic Acid	Railcar	Fertilizer
60	CO Purchase	Formic Acid	Railcar	FCEV vehicle filling
61	CO Purchase	Methanol	Pipeline	Fertilizer
62	CO Purchase	Methanol	Pipeline	FCEV vehicle filling
63	CO Purchase	Methanol	Railcar	Fertilizer
64	CO Purchase	Methanol	Railcar	FCEV vehicle filling

### III. Supplemental Analysis - Feedstock Price Perturbation

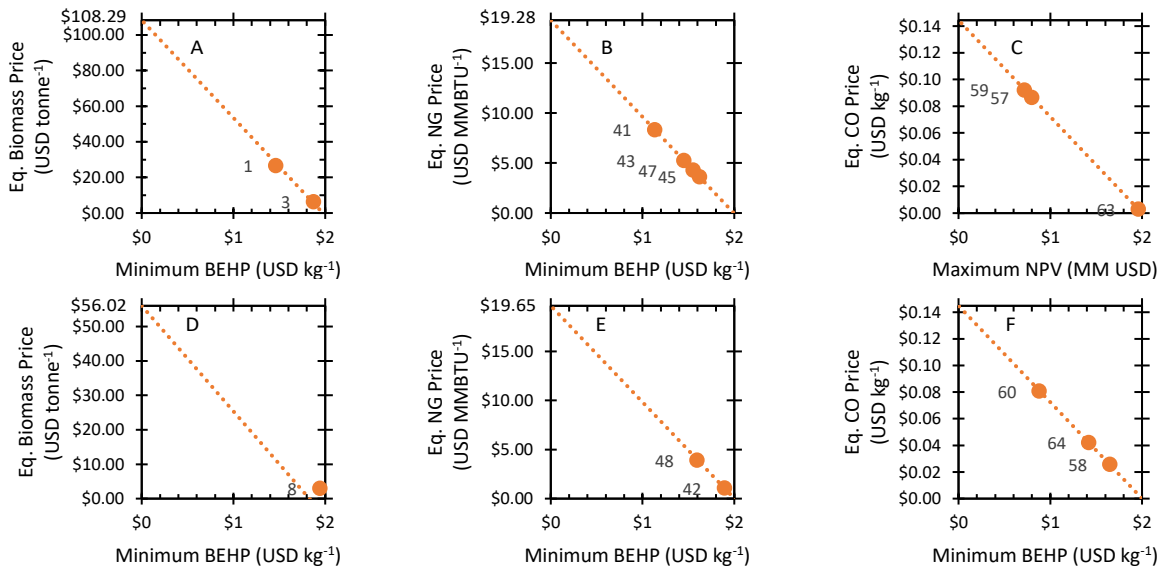
The default scenarios, 1 through 64, utilise commodity price data found in government databases, techno-economic analyses, and market data hubs. Similarly, as discussed in the previous section, the changes in the price of the feedstocks can significantly alter the economic viability of a business case. This section analyses the effect of increasing, and occasionally decreasing, the purchase price of these commodities to visualise how future market fluctuations can potentially disturb the hydrogen business.

Figure SA1 shows key parameters of the 25-year NPV functions for all non-electrolyser supply chains. These NPV functions are derived from at least four feedstock price points (scenarios 1-12, 41-64, 129-132, 161-196, and 225-248), starting at zero then low, medium, and high. When segregated by production technology and end-use, there is an interesting linear trend that appears when the maximum NPV is plotted against the break-even feedstock price. This trend correlates supply chains with different storage mediums and transportation methods, indicating that the rate of NPV appreciation depends only on the production method and end-use. The storage medium and transportation method seem to only affect the maximum achievable NPV and does not change the relationship between NPV and feedstock price. This is a peculiar result since there appears to be no obvious connection between those supply chains. Nevertheless, the result makes determining break-even feedstock prices very predictable, as any new supply chain may be classified into any of the six groups in Figure SA1 and the break-even feedstock price can be determined from the NPV of the zero-cost business.

Similarly, the BEHP can also be grouped into the same six groups. Figure SA2 shows the minimum achievable BEHP for each supply chain. Using the feedstock price correlation shown in Figure S6, one can determine the price necessary to reach a BEHP of 2.00 USD kg<sup>-1</sup> can be determined by the X-intercept. This equivalent feedstock price is plotted on the vertical axis of Figure SA2 to show the linear relationship for each class of supply chains. In plots A, D, and E, most supply chains are not able to reach the desired BEHP. Despite this, they still correlate with the other data to create a strong regression line. The Y-intercept of this line shows the maximum feedstock price for each class that can still break-even selling hydrogen at the aforementioned price. The Y-intercepts



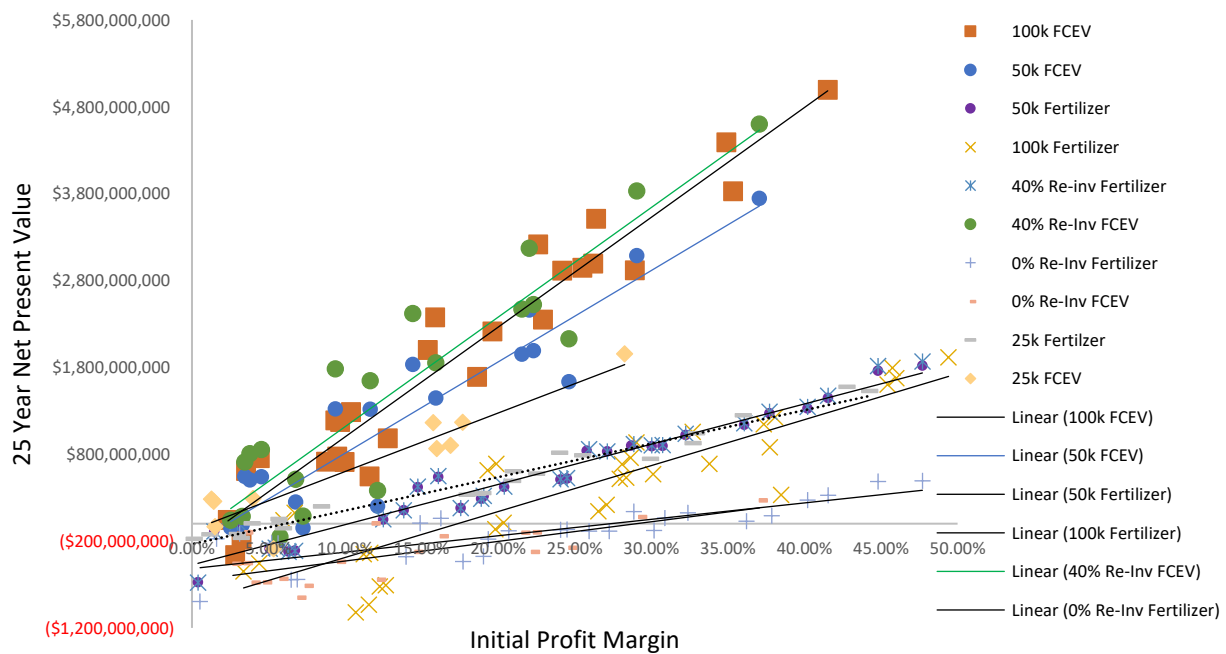
**Figure SA1** 25-year net present value functions, separated by feedstock type and end-use. A feedstock price of zero provides the maximum achievable NPV, plotted against the break-even feedstock price to achieve a positive NPV. Each point is labelled with the respective supply chain. (A) Wood BG-Fertiliser Manufacturing (B) Wood BG-FCEV Filling (C) SMR-Fertiliser Manufacturing (D) SMR-FCEV Filling (E) CO Purchase-Fertiliser Manufacturing (F) CO Purchase-FCEV Filling. Supply chain 6 is not shown on the B plot because its maximum NPV is negative.



**Figure SA2** Break-even hydrogen price functions, separated by feedstock type and end-use. A feedstock price of zero provides the minimum achievable BEHP, plotted against the minimum feedstock price needed to achieve a BEHP of 2.00 USD kg<sup>-1</sup>. Each point is labelled with the respective supply chain. (A) Wood BG-Fertiliser Manufacturing (B) Wood BG-FCEV Filling (C) SMR-Fertiliser Manufacturing (D) SMR-FCEV Filling (E) CO Purchase-Fertiliser Manufacturing (F) CO Purchase-FCEV Filling. Points not shown on the plot have negative equivalent feedstock prices.

indicate that the change in end-use does not have a significant effect; only plot 21A and 21D display a major difference. Furthermore, the latter's weaker regression ( $R^2 = 0.9743$ ) is significantly more variable than the next sparse regression ( $R^2 = 0.9996$ ), so the difference should be questioned. This is mainly due to an outlier, supply chain 4 at point (5.34, -103.38), which has a high leverage and pulls the Y-intercept of the regression down. Excluding this outlier, the Y-intercept and regression coefficient become 94.84 USD tonne<sup>-1</sup> and 0.9864 respectively, approaching the regression of plot 21A. Despite the results from a two-sample t-test indicating that only 21C and 21F are statistically identical using 95% confidence, the effect of varying the end-use is negligible in each case.

### III. Supplemental Figures



**Figure S1.** NPV achieved for various scaling strategies, plotted against the respective initial profit margin.

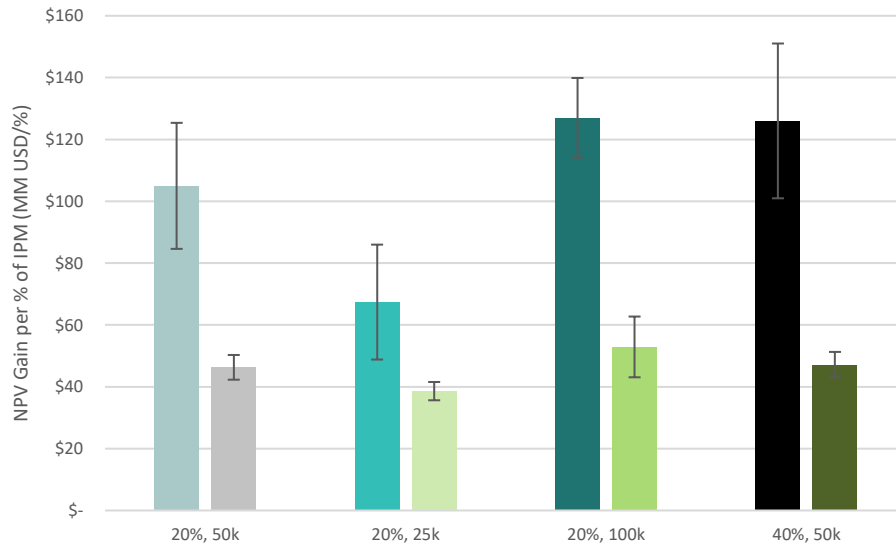


Figure S2. Slope of NPV as a function of Initial Profit Margin (IPM). Shown with regression confidence intervals and split into experimental groups. [end-use, initial daily production, reinvestment rate]: FCEV, 50k, 40% (**olive**); FCEV, 100k, 20% (**green**); FCEV, 50k, 20% (**grey**); FCEV, 25k, 20% (**light green**); Fert., 25k, 20% (**cyan**); Fert., 50k, 20% (**pale blue**); Fert., 50k, 40% (**black**); Fert., 100k, 20% (**dark blue**).

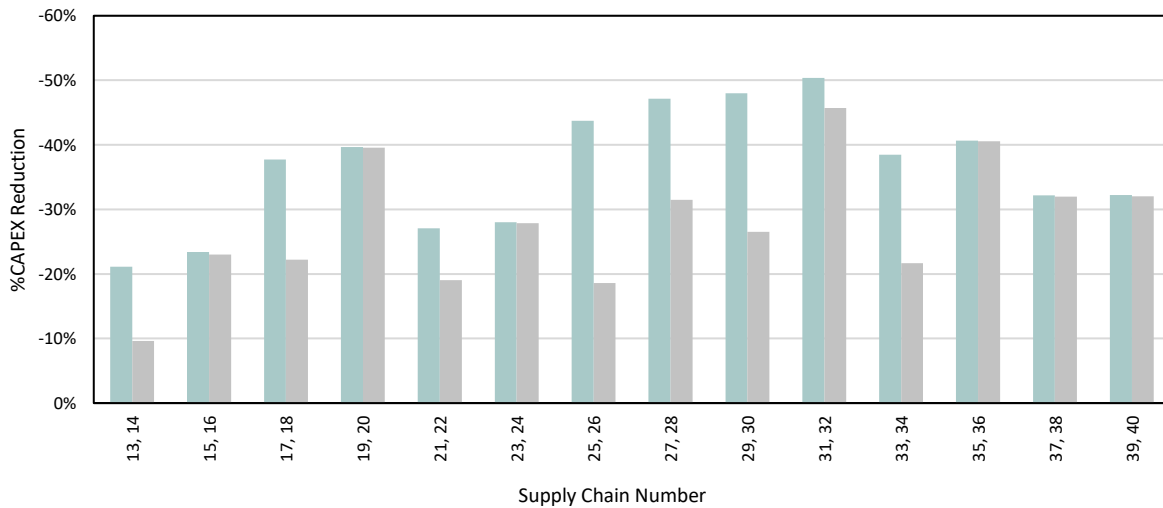


Figure S3. Reduction in total overnight cost for each electrolyser supply chain. Fertiliser supply chains are shown in **pale blue** and FCEV filling supply chains are shown in **grey**.



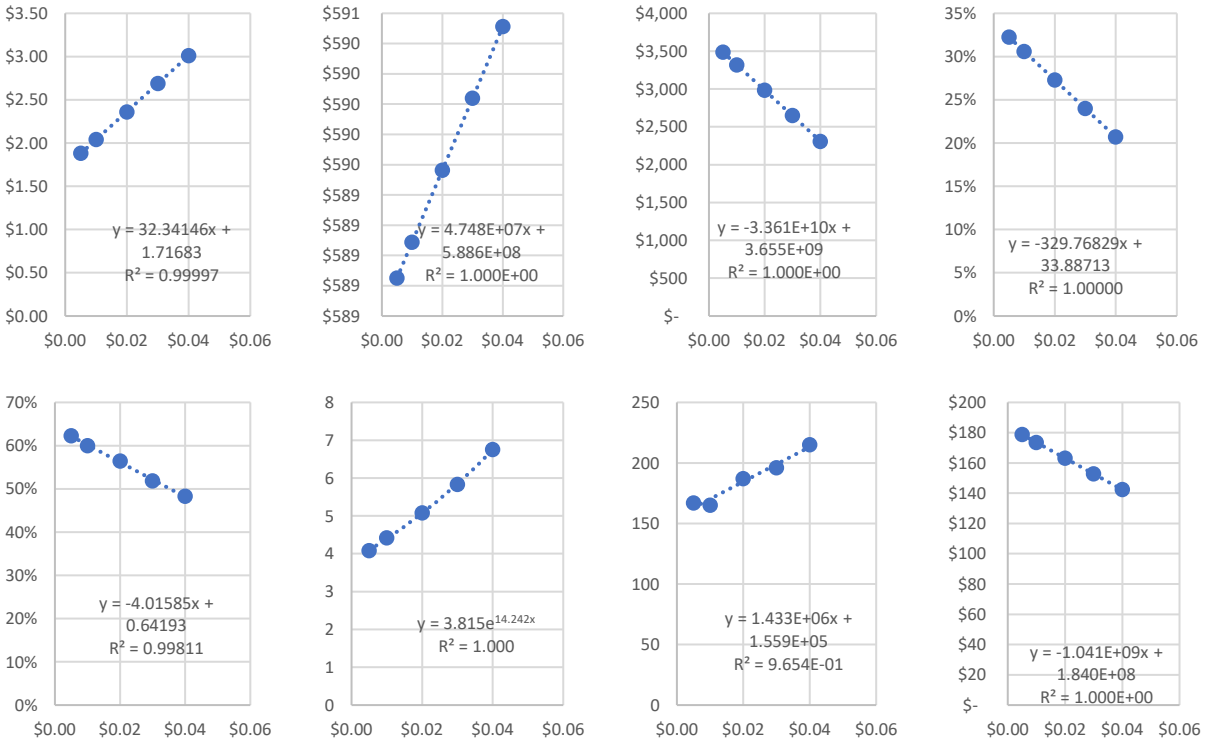


Figure S4. Business properties of supply chain 20 as a function of electricity price during 23-hour operation strategy: **A.** Break-even hydrogen price; **B.** Total overnight cost (MM USD); **C.** Net present value (MM USD); **D.** Initial profit margin; **E.** Max profit margin; **F.** Payback period; **G.** Minimum profitable production scale (x 10<sup>3</sup> kg/day); **H.** Monthly EBITDA at year 25 (MM USD).

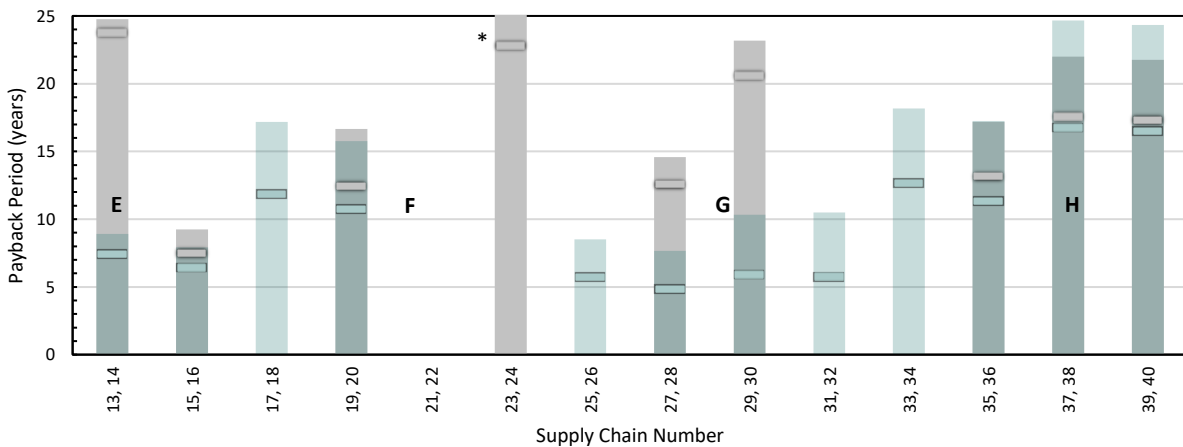


Figure S5. Payback period comparison between the default electrolyser scenarios (bars) and the 0.04 USD/kWh electricity purchasing scenario using the 23-hour strategy. Supply chains that do not achieve a payback period less than 25 years with either strategy are not shown. \*PBP for supply chain 24 is greater than 25 years.

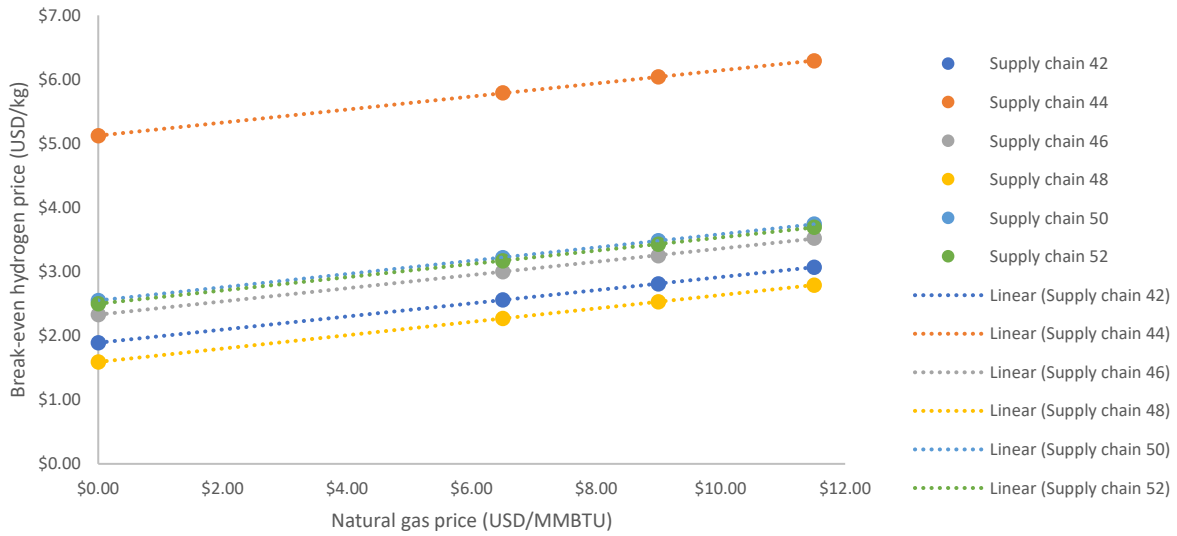


Figure S6. Example of linear regression of BEHP vs. price for SMR supply chains.

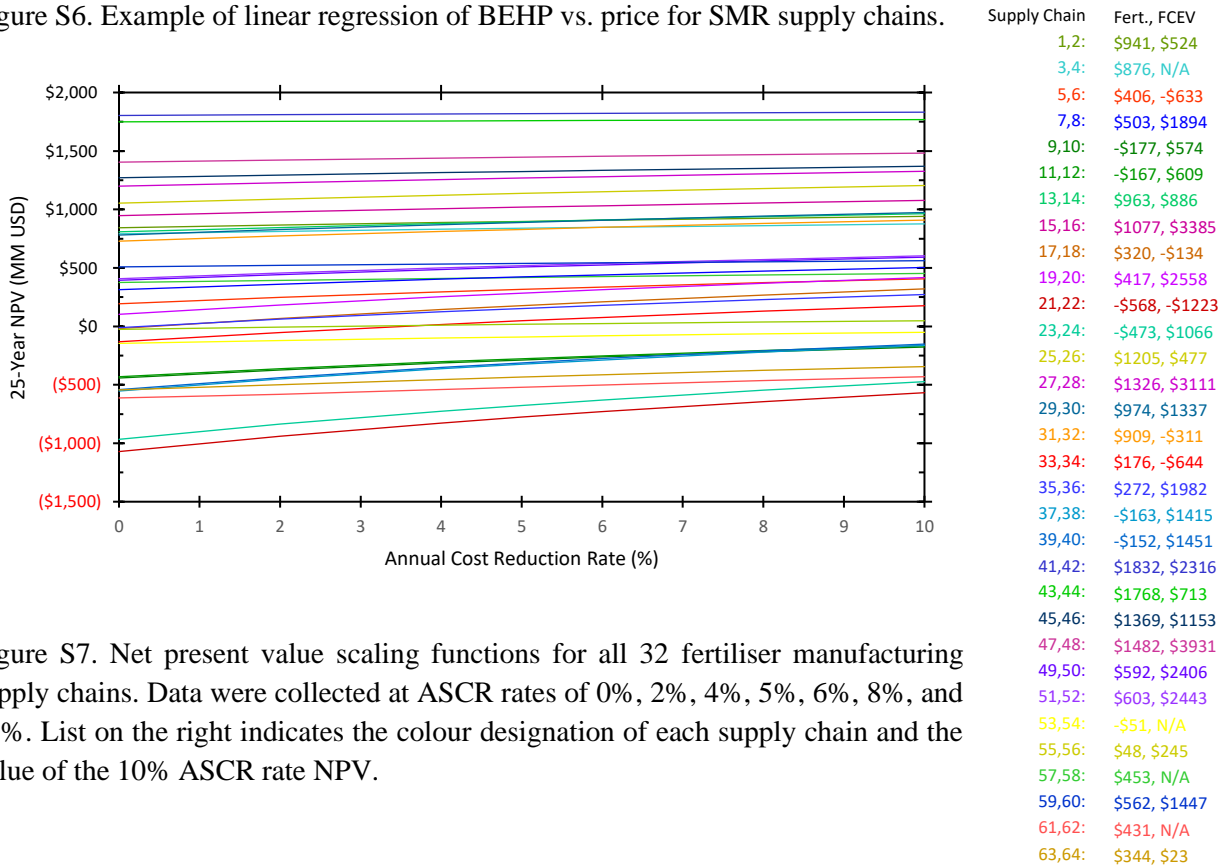


Figure S7. Net present value scaling functions for all 32 fertiliser manufacturing supply chains. Data were collected at ASCR rates of 0%, 2%, 4%, 5%, 6%, 8%, and 10%. List on the right indicates the colour designation of each supply chain and the value of the 10% ASCR rate NPV.

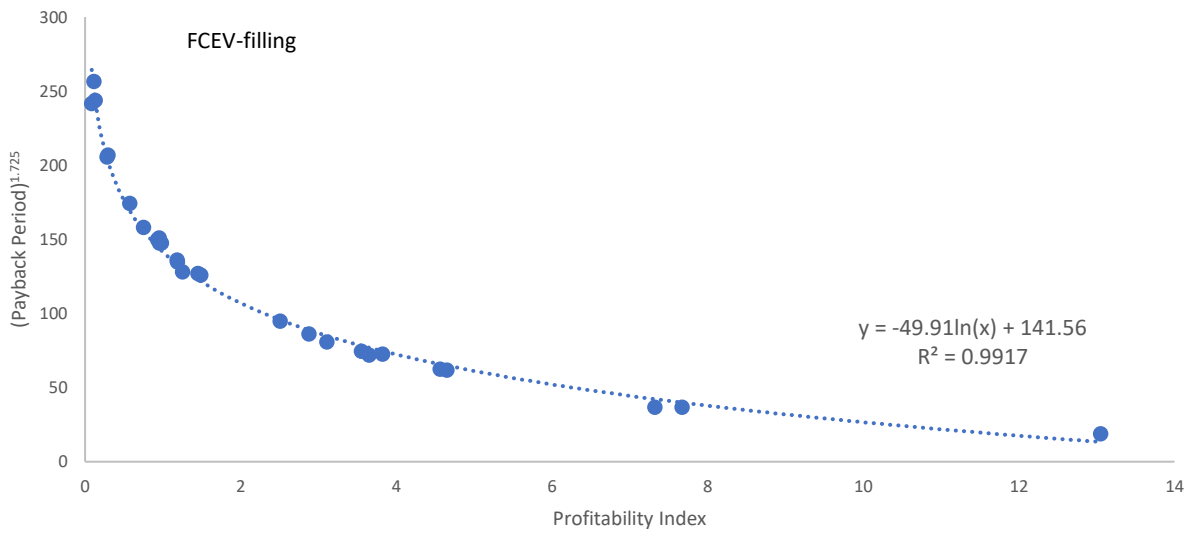
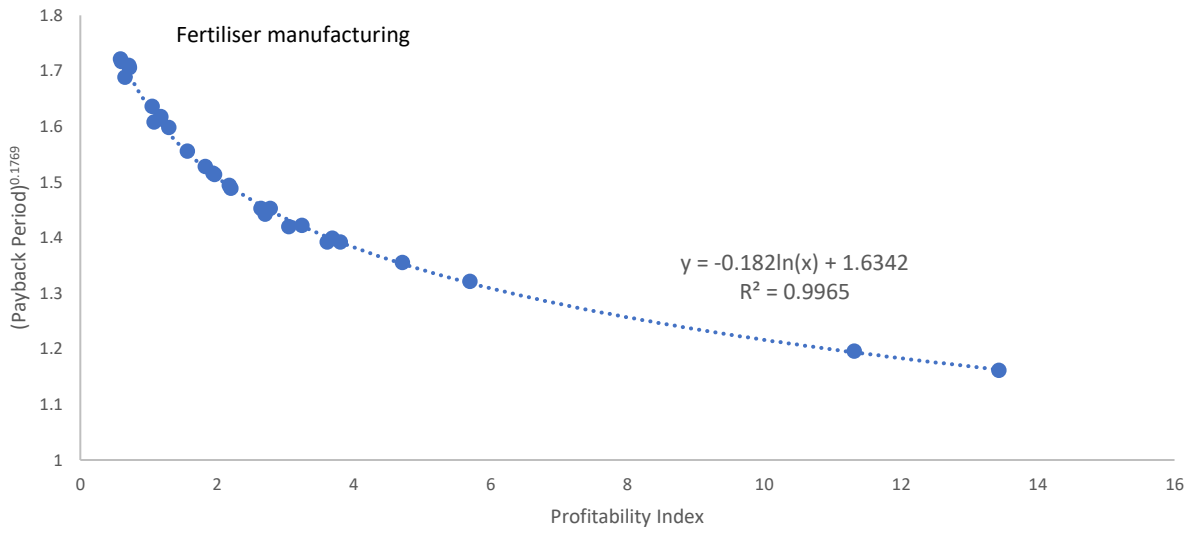


Figure S8. Correlation between profitability index and the supply chain’s payback period. The parity between payback period exponents indicates the sensitivity of the payback period to the business case’s PI, where fertiliser manufacturing is more sensitive to changes in PI.

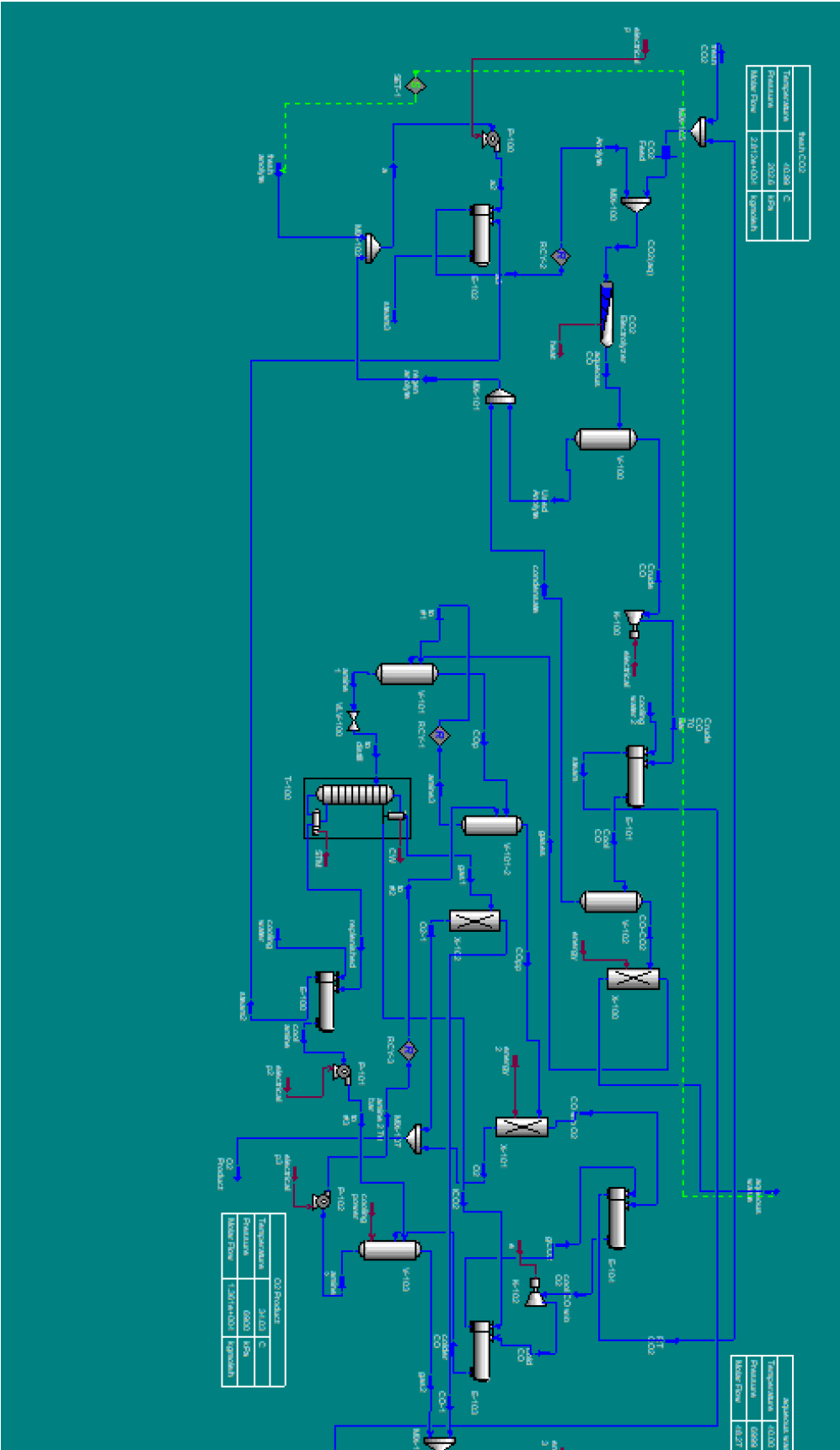


Figure S9. UniSim Design process flow diagram for a CO<sub>2</sub> electrolysis to formic acid supply chain. Electricity generation and transportation equipment not shown. Inlet streams include carbon dioxide, electrolyser analyte, methanol, and water. Outlet streams include aqueous waste, oxygen, methyl formate-rich gas, methanol recycle, and formic acid.

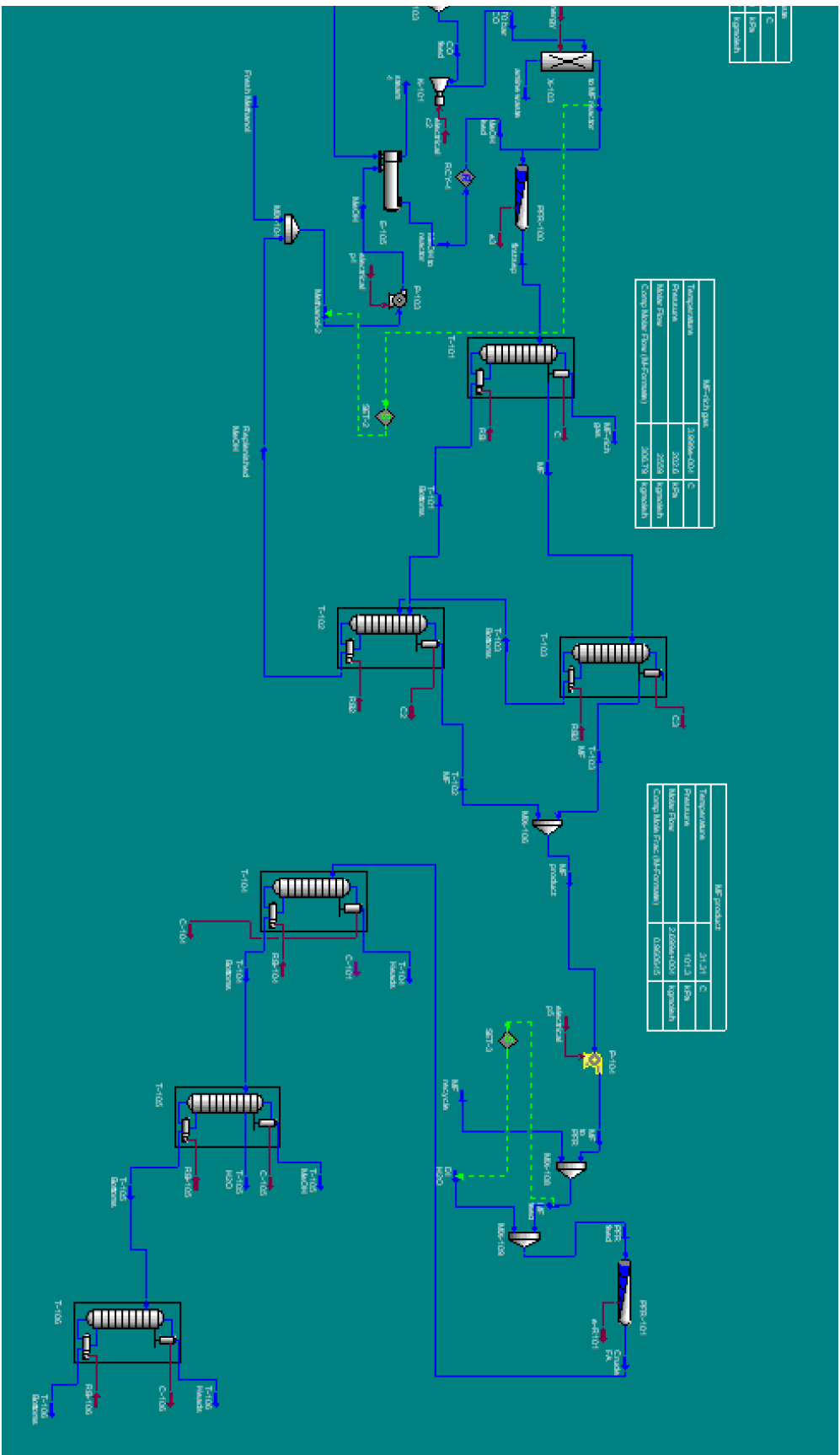


Figure S9. UniSim Design process flow diagram for a CO<sub>2</sub> electrolysis to formic acid supply chain. Electricity generation and transportation equipment not shown. Inlet streams include carbon dioxide, electrolyser analyte, methanol, and water. Outlet streams include aqueous waste, oxygen, methyl formate-rich gas, methanol recycle, and formic acid.

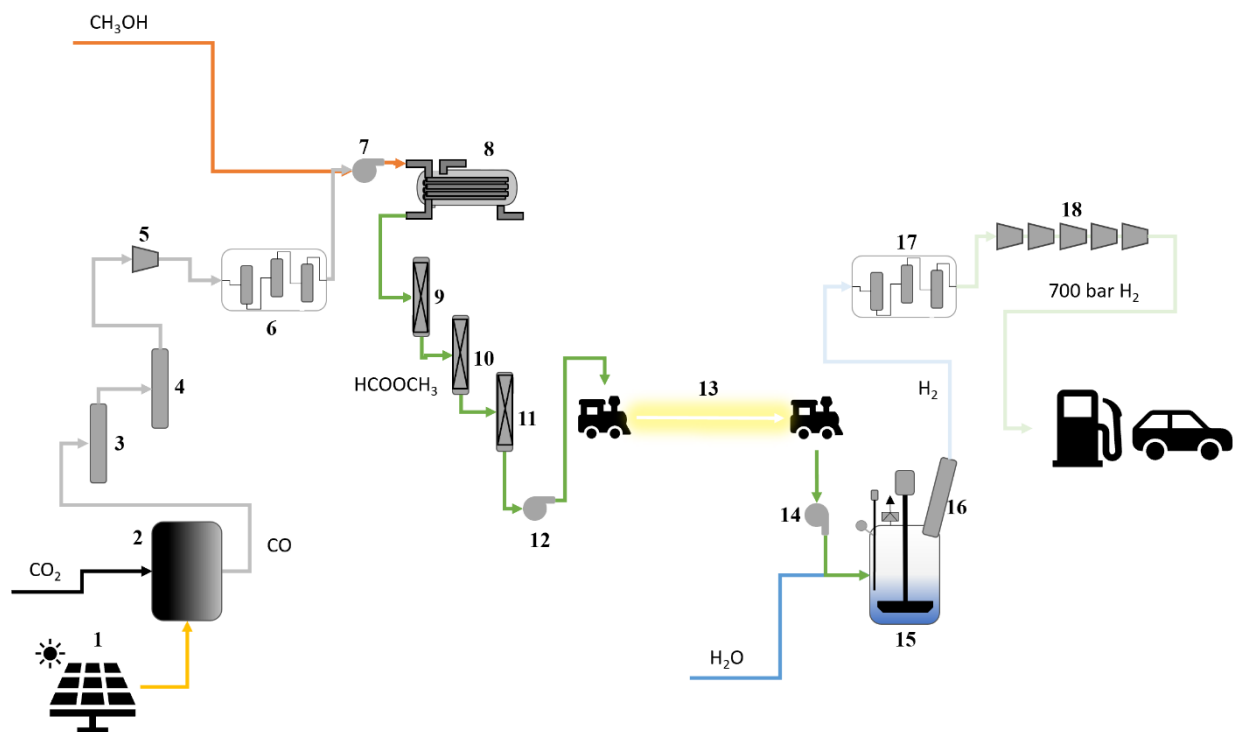


Figure S10. Simplified process flow diagram of supply chain **16**. All equipment items and processes costed in HBAT are listed with exceptions. For simplicity, heat exchangers, storage tanks, and recycle streams are not shown but are also accounted for. Production: PV-coupled CO<sub>2</sub> electrolysis; storage: methyl formate; transportation: railcar; end-use: FCEV filling.

Table S3. Example equipment list for supply chain **16**.

Identifier #	Equipment Item	Bare Module Cost (x10 <sup>3</sup> USD)
<b>1</b>	PV Solar Arrays	53,000
<b>2</b>	CO <sub>2</sub> Electrolyser	43,000
<b>3</b>	Flash Vessel	50
<b>4</b>	Flash Vessel	50
<b>5</b>	Generic Compressor	1,703
<b>6</b>	Sweet/Sour Amine Seps.	57,000
<b>7</b>	Positive Displacement Pump	173
<b>8</b>	Plug-Flow Methanol Carbonylation Reactor	4,415
<b>9</b>	Distillation Column	433
<b>10</b>	Distillation Column	433
<b>11</b>	Distillation Column	433
<b>12</b>	Positive Displacement Pump	173
<b>13</b>	Methyl Formate Railcars	280
<b>14</b>	Positive Displacement Pump	173
<b>15</b>	Methyl Formate Dehydrogenation Reactor	107,000
<b>16</b>	Reflux Condenser	253
<b>17</b>	Pressure-Swing Adsorption Seps.	9,962
<b>18</b>	Five-Stage FCEV H <sub>2</sub> Compressors	4,617

Table S4. ASCR optimization results. Red highlight indicates negative NPV scenario.

Supply Chain #	Max R&D Annual Benefit per Point	Optimal ASCR (%)	Total Annual Benefit
1	\$ 10,719,677	2	\$ 21,439,355
2	\$ 49,069,586	10	\$ 490,695,858
3	\$ 9,333,618	2	\$ 18,667,236
4	\$ 25,481,437	2	\$ 50,962,875
5	\$ 53,171,108	10	\$ 531,711,077
6	\$ 22,361,748	2	\$ 44,723,496
7	\$ 194,359,253	2	\$ 388,718,506
8	\$ 32,061,843	2	\$ 64,123,687
9	\$ 53,774,221	10	\$ 537,742,211
10	\$ 32,052,356	2	\$ 64,104,712
11	\$ 57,066,772	10	\$ 570,667,720
12	\$ 17,446,766	2	\$ 34,893,532
13	\$ 82,955,333	10	\$ 829,553,328
14	\$ 14,455,823	2	\$ 28,911,647
15	\$ 116,283,667	2	\$ 232,567,334
16	\$ 33,665,922	4	\$ 134,663,689
17	\$ 137,717,553	10	\$ 1,377,175,530
18	\$ 37,634,931	2	\$ 75,269,862
19	\$ 313,592,845	2	\$ 627,185,691
20	\$ 61,190,095	2	\$ 122,380,191
21	\$ 72,118,458	10	\$ 721,184,579
22	\$ 60,544,701	2	\$ 121,089,401
23	\$ 99,827,371	10	\$ 998,273,707
24	\$ 16,635,518	2	\$ 33,271,037
25	\$ 44,651,137	10	\$ 446,511,375
26	\$ 13,831,835	2	\$ 27,663,670
27	\$ 283,922,177	2	\$ 567,844,353
28	\$ 21,839,227	2	\$ 43,678,454
29	\$ 125,206,062	10	\$ 1,252,060,624
30	\$ 20,397,915	2	\$ 40,795,829
31	\$ 45,425,268	10	\$ 454,252,679
32	\$ 16,512,862	10	\$ 165,128,620
33	\$ 86,858,150	10	\$ 868,581,499
34	\$ 29,120,184	4	\$ 116,480,737
35	\$ 275,801,069	2	\$ 551,602,139
36	\$ 48,230,851	2	\$ 96,461,703
37	\$ 132,536,830	10	\$ 1,325,368,301
38	\$ 48,075,372	2	\$ 96,150,744
39	\$ 135,913,639	10	\$ 1,359,136,387
40	\$ 2,860,030	2	\$ 5,720,061
41	\$ 267,564,565	2	\$ 535,129,130
42	\$ 1,944,547	2	\$ 3,889,094

<b>43</b>	\$	74,174,346	2	\$	148,348,692
<b>44</b>	\$	10,590,074	2	\$	21,180,148
<b>45</b>	\$	108,054,420	10	\$	1,080,544,203
<b>46</b>	\$	8,197,257	2	\$	16,394,513
<b>47</b>	\$	69,692,405	2	\$	139,384,810
<b>48</b>	\$	23,145,056	2	\$	46,290,112
<b>49</b>	\$	197,959,188	2	\$	395,918,376
<b>50</b>	\$	22,949,684	2	\$	45,899,368
<b>51</b>	\$	194,812,158	2	\$	389,624,316
<b>52</b>	\$	11,579,222	2	\$	23,158,444
<b>53</b>					
<b>54</b>	\$	4,456,026	10	\$	44,560,256
<b>55</b>	\$	22,960,153	10	\$	229,601,528
<b>56</b>	\$	8,724,343	2	\$	17,448,686
<b>57</b>					
<b>58</b>	\$	5,802,588	2	\$	11,605,175
<b>59</b>	\$	50,207,512	2	\$	100,415,024
<b>60</b>	\$	17,437,648	6	\$	104,625,889
<b>61</b>					
<b>62</b>	\$	20,920,996	4	\$	83,683,983
<b>63</b>	\$	52,064,201	10	\$	520,642,009
<b>64</b>	\$	10,719,677	2	\$	21,439,355



#### IV. Data sources and references

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Data Acquired for Selected Counties	Data Source
Market Availability	1-5
Market Size	1-5
Consumption of Hydrogen	1-3
Cost of Water/Water Treatment	4
Supply of Clean Energy	11, 14, 18-29
Real Estate Cost	30-33
Current Price of Oil	34
Current Price of Local Gasoline	35-38
Current Price of Local Electricity	7-17
Current Price of Steel	39-40
Government Incentives	41-45
Emissions	1, 6
Public opinion	Online polling
Technical data	46-86

1. A. Elgowainy, M. Mintz, U. Lee, T. Stephens, P. Sun, K. Reddi, Y. Zhou, G. Zang, M. Ruth, P. Jadun, E. Connelly, R. Boardman. Assessment of Potential Future Demands for Hydrogen in the United States. 2020, Argonne National Laboratory.
2. U.S. Department of Energy. 2016. *2016 Billion-Ton Report: Advancing Domestic Resources for a Thriving Bioeconomy, Volume 1: Economic Availability of Feedstocks*. M. H. Langholtz, B. J. Stokes, and L. M. Eaton (Leads), ORNL/TM-2016/160. Oak Ridge National Laboratory, Oak Ridge, TN. 448p. doi: 10.2172/1271651. <http://energy.gov/eere/bioenergy/2016-billion-ton-report>.
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