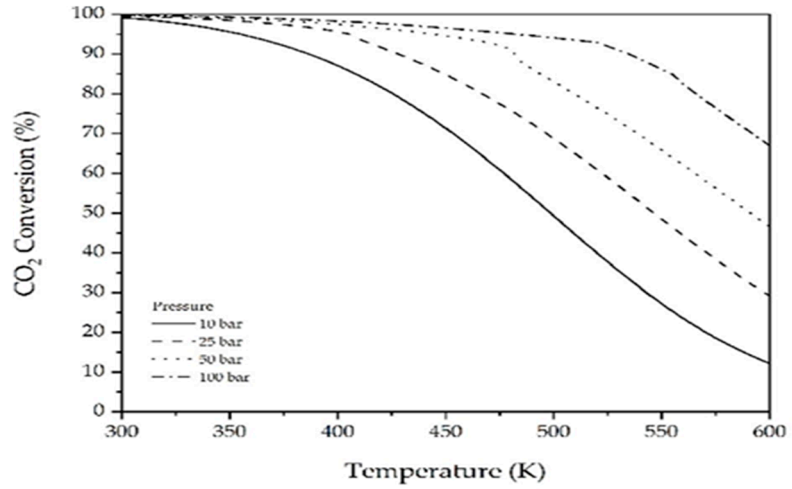


Figure S1: Effects of Temperature and Pressure on CO_2 Conversion [31]

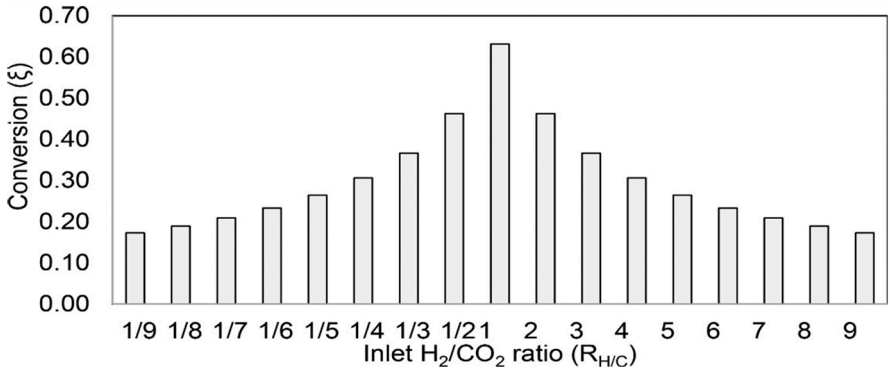


Figure 8. Initial H $_2$/CO $_2$ ratio in fl uence on the reaction conversion.

Figure S2: Correlation between Reaction Yield and H_2/CO_2 Input Ratio [31]

SUPPLEMETARY INFORMATION

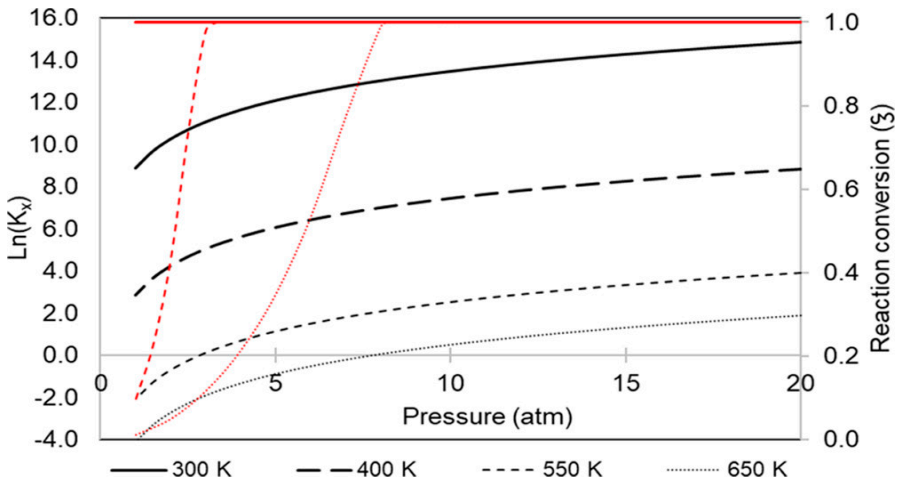


Figure S3 : Influence of the temperature and pressure on the reaction conversion and equilibrium constant [31].

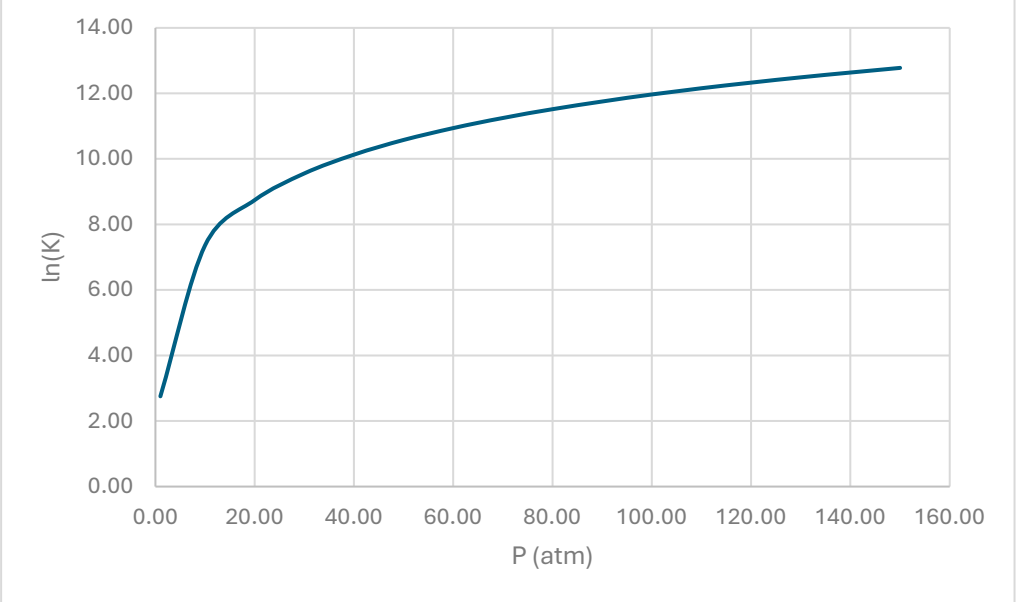


Figure S4 : Dependence of the equilibrium constant on pressure at 300 K, calculated from the extended van't Hoff relation [31].

SUPPLEMETARY INFORMATION

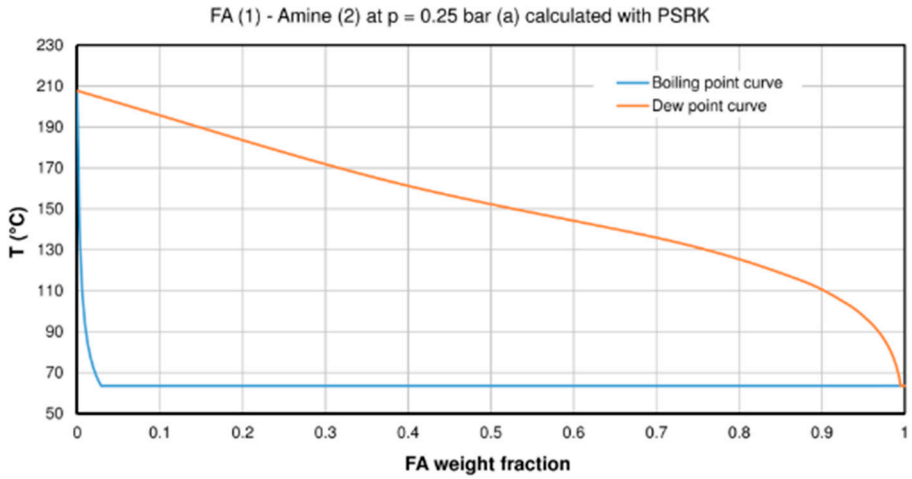


Figure S5: phase diagram for the mixture formic acid-trihexylamine [30]

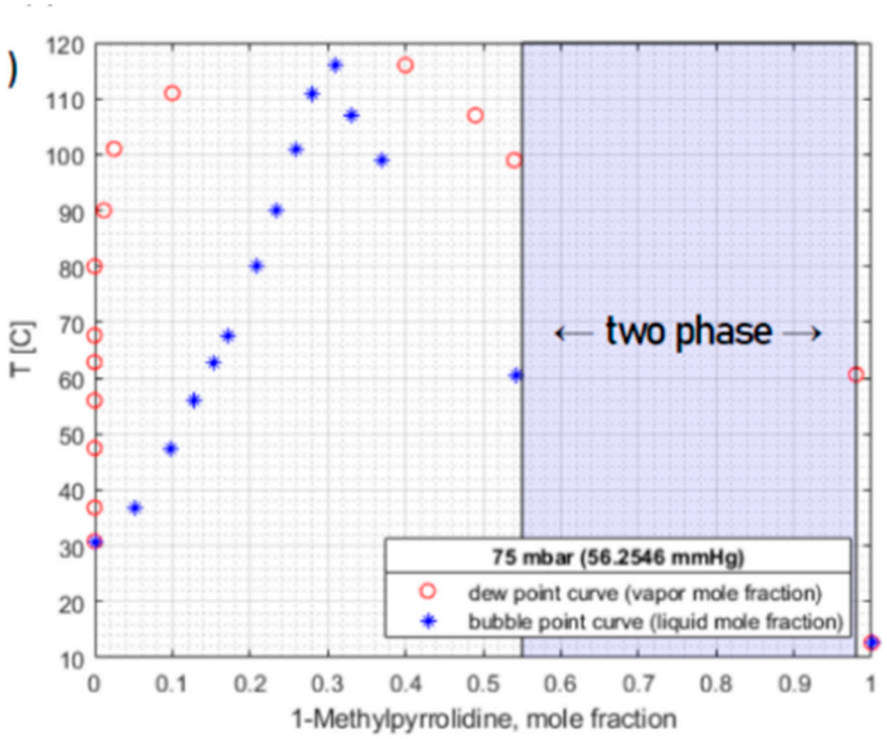


Figure S6: Vapor-Liquid equillibrium for Formic acid-NMPI [20]

SUPPLEMETARY INFORMATION

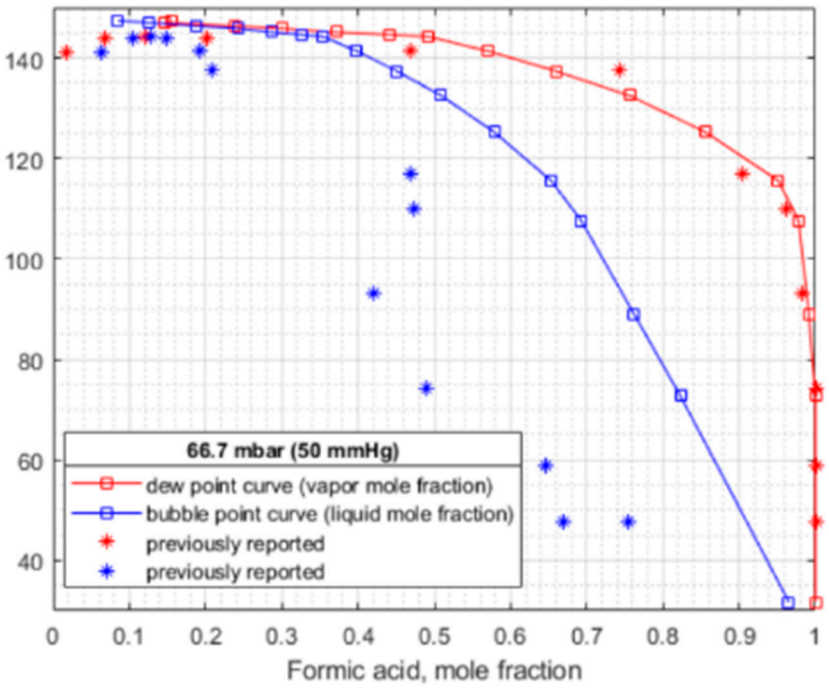


Figure S7: Vapor-Liquid equillibrium for Formic acid-N [20]

SUPPLEMETARY INFORMATION

Table S1. Operating conditions and mass flow rates of major components in Section 100 of case study A.

Stream	**S-101**	**S-102**	**S-103**	**S-104**	**S-105**	**S-106**	**S-107**	**S-108**
Total Mass Flow (kg/h)	1611.00	103.24	12.01	10.00	1611.00	2171.02	2171.02	103.24
Temperature (°C)	25.00	25.00	25.00	25.00	53.73	78.20	34.21	112.25
Pressure (bar)	70.00	30.00	1.01	1.01	104.00	104.00	104.00	70.00
Component Mass Flow (kg/h)								
CO_2	1611.00	0.00	0.00	0.00	1611.00	1889.62	1889.62	0.00
Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Formic Acid	0.00	0.00	0.00	0.00	0.00	0.01	0.01	0.00
H_2	0.00	103.24	0.00	0.00	0.00	277.71	277.71	103.24
Methanol	0.00	0.00	0.00	0.00	0.00	3.69	3.69	0.00
Catalyst	0.00	0.00	0.00	0.35	0.00	0.00	0.00	0.00
Trihexylamine	0.00	0.00	0.00	9.65	0.00	0.00	0.00	0.00
Water	0.00	0.00	12.01	0.00	0.00	0.00	0.00	0.00

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Table S2. Operating conditions and mass flow rates of major components in Section 100 of case study A.

Stream	**S-109**	**S-110**	**S-111**	**S-112**	**S-113**	**S-114**	**S-115**	**S-116**
Total Mass Flow (kg/h)	103.24	103.24	103.24	2274.26	12.01	12.01	17379.43	17379.43
Temperature (°C)	35.00	75.48	35.00	34.37	25.00	27.66	97.74	97.74
Pressure (bar)	70.00	105.00	105.00	104.00	1.01	105.01	0.04	1.01
Component Mass Flow (kg/h)								
CO_2	0.00	0.00	0.00	1889.62	0.00	0.00	0.00	0.00
Complex	0.00	0.00	0.00	0.00	0.00	0.00	45.39	45.39
Formic Acid	0.00	0.00	0.00	0.01	0.00	0.00	1.84	1.84
H_2	103.24	103.24	103.24	380.94	0.00	0.00	0.00	0.00
Methanol	0.00	0.00	0.00	3.69	0.00	0.00	284.52	284.52
Catalyst	0.00	0.00	0.00	0.00	0.00	0.00	0.85	0.85
Trihexylamine	0.00	0.00	0.00	0.00	0.00	0.00	17045.33	17045.33
Water	0.00	0.00	0.00	0.00	12.01	12.01	1.50	1.50

Table S3. Operating conditions and mass flow rates of major components in Section 100 of case study A.

Stream	**S-117**	**S-118**	**S-119**	**S-120**	**S-121**	**S-122**	**S-123**
Total Mass Flow (kg/h)	7130.82	10248.62	10248.62	10248.62	14157.18	3896.55	560.02
Temperature (°C)	97.74	97.74	25.00	34.25	32.33	29.70	86.44
Pressure (bar)	1.01	1.01	1.01	105.01	105.00	105.00	134.00
Component Mass Flow (kg/h)							
CO_2	0.00	0.00	0.00	0.00	0.00	0.00	278.62
Complex	18.63	26.77	26.77	26.77	26.77	0.00	0.00
Formic Acid	0.76	1.09	1.09	1.09	52.39	51.31	0.01
H_2	0.00	0.00	0.00	0.00	0.00	0.00	277.71
Methanol	116.74	167.78	167.78	167.78	3256.15	3088.37	3.69
Catalyst	0.35	0.50	0.50	0.50	0.50	0.00	0.00
Trihexylamine	6993.73	10051.60	10051.60	10051.60	10051.60	0.00	0.00
Water	0.61	0.88	0.88	0.88	769.77	756.88	0.00

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Table S4. Operating conditions and mass flow rates of major components in Section 200 of case study A.

Stream	**S-201**	**S-202**	**S-203**	**S-204**	**S-205**	**S-206**	**S-207**
Total Mass Flow (kg/h)	16431.44	16424.67	721.49	15703.18	622.25	560.02	62.22
Temperature (°C)	32.84	93.00	91.72	91.72	35.00	35.00	35.00
Pressure (bar)	104.00	104.00	80.00	80.00	80.00	80.00	80.00
Component Mass Flow (kg/h)							
CO_2	1889.62	309.57	309.57	0.00	309.57	278.62	30.96
Complex	26.77	11348.71	0.10	11348.60	0.00	0.00	0.00
Formic Acid	52.40	52.40	0.45	51.95	0.01	0.01	0.00
H_2	380.94	308.56	308.56	0.00	308.56	277.71	30.86
Methanol	3259.84	3259.84	96.30	3163.54	4.10	3.69	0.41
Catalyst	0.50	0.50	0.00	0.50	0.00	0.00	0.00
Trihexylamine	10051.59	375.31	0.00	375.31	0.00	0.00	0.00
Water	769.77	769.77	6.49	763.27	0.00	0.00	0.00

Table S5. Operating conditions and mass flow rates of major components in Section 300 of case study A.

Stream	S-301	S-302	S-303	S-304	S-305	S-306
Total Mass Flow (kg/h)	15802.42	15802.42	15802.42	329.64	15472.78	16218.76
Temperature (°C)	90.72	40.00	45.30	45.30	45.30	36.73
Pressure (bar)	80.00	80.00	130.00	130.00	130.00	1.01
Component Mass Flow (kg/h)						
CO_2	0.00	0.00	0.00	0.00	0.00	0.00
Complex	11348.71	11348.71	11348.71	0.00	11348.71	11348.71
Formic Acid	52.39	52.39	52.39	0.00	52.39	52.39
H_2	0.00	0.00	0.00	0.00	0.00	0.00
Methanol	3255.74	3255.74	3255.74	127.18	3128.56	2971.22
Catalyst	0.50	0.50	0.50	0.29	0.21	0.11
Trihexylamine	375.31	375.31	375.31	202.17	173.15	1076.57
Water	769.77	769.77	769.77	0.00	769.77	769.77

Table S6. Operating conditions and mass flow rates of major components in Section 300 of case study A.

Stream	**S-306**	**S-307**	**S-308**	**S-309**	**S-310**	**S-311**	**S-312**	**S-313**
Total Mass Flow (kg/h)	6254.02	6583.66	3785.38	3785.38	140.00	3925.38	3896.55	28.83
Temperature (°C)	36.73	37.26	71.49	25.00	25.00	25.00	25.00	25.00
Pressure (bar)	1.01	1.01	1.00	1.00	1.01	1.00	1.00	1.00
Component Mass Flow (kg/h)								
CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Formic Acid	0.00	0.00	51.68	51.68	0.00	51.68	51.31	0.38
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol	157.34	284.52	2971.22	2971.22	140.00	3111.22	3088.37	22.85
Catalyst	0.10	0.40	0.00	0.00	0.00	0.00	0.00	0.00
Trihexylamine	6096.58	6298.75	0.00	0.00	0.00	0.00	0.00	0.00
Water	0.00	0.00	762.48	762.48	0.00	762.48	756.88	5.60

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Table S7. Operating conditions and mass flow rates of major components in Section 400 of case study A.

Stream	**S-401**	**S-402**	**S-403**	**S-404**	**S-405**	**S-406**	**S-407**	**S-408**	**S-409**	**S-410**
Total Mass Flow (kg/h)	0.00	12433.38	12433.38	12440.15	1654.38	1654.38	0.00	0.00	0.00	17369.43
Temperature (°C)	25.00	175.25	180.00	83.93	15.23	15.29	25.00	25.00	25.00	97.78
Pressure (bar)	1.01	0.25	0.25	0.25	0.04	1.01	1.01	1.01	1.01	0.04
	Component Mass Flow (kg/h)									
CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	284.52
Formic Acid	0.00	0.11	0.11	0.11	0.00	0.00	0.00	0.00	0.00	0.50
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Methanol	0.00	7.29	7.29	7.29	5.79	5.79	0.00	0.00	0.00	1.50
Catalyst	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	284.52
Trihexylamine	0.00	0.11	0.11	0.11	0.00	0.00	0.00	0.00	0.00	0.50
Water	0.00	1076.57	1076.57	10736.93	0.00	0.00	0.00	0.00	0.00	17035.68

Table S8. Operating conditions and mass flow rates of major components in Section 100 of case study B.

Stream	**S-101**	**S-102**	**S-103**	**S-104**	**S-105**	**S-106**	**S-107**	**S-108**	**S-109**
Total Mass Flow (kg/h)	1612.85	76.00	4.80	9.79	1612.85	76.00	76.00	76.00	4.80
Temperature (°C)	25	25	25	25	65	128	35	75	25
Pressure (bar)	70.00	30.00	1.01	1.01	120.00	80.00	80.00	120.00	1.01
Component Mass Flow (kg/h)									
CO_2	1612.85	0.00	0.00	0.00	1612.85	0.00	0.00	0.00	0.00
H_2	0.00	76.00	0.00	0.00	0.00	76.00	76.00	76.00	0.00
NMPI	0.00	0.00	4.80	0.00	0.00	0.00	0.00	0.00	4.80
NMPI-FA Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	0.00	0.00	0.00	9.79	0.00	0.00	0.00	0.00	0.00

Table S9. Operating conditions and mass flow rates of major components in Section 100 of case study B.

Stream	**S-110**	**S-111**	**S-112**	**S-113**	**S-114**	**S-115**	**S-116**
Total Mass Flow (kg/h)	4.80	9.79	9.79	4.80	5.00	9.80	0.00
Temperature (°C)	33	25	28	28	28	30	25
Pressure (bar)	120.01	1.01	120.01	120.01	120.01	120.01	1.01
Component Mass Flow (kg/h)							
CO_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NMPI	4.80	0.00	0.00	0.00	0.00	4.80	0.00
NMPI-FA Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	0.00	9.79	9.79	4.80	5.00	5.00	0.00

Table S10. Operating conditions and mass flow rates of major components in Section 100 of case study B.

Stream	**S-117**	**S-118**	**S-119**	**S-120**	**S-121**	**S-122**	**S-123**
Total Mass Flow (kg/h)	7495.13	3.75	7491.38	7496.18	7505.98	1688.84	9194.82
Temperature (°C)	37	37	37	37	37	70	40
Pressure (bar)	120.07	120.07	120.07	120.01	120.01	120.00	120.00
Component Mass Flow (kg/h)							
CO_2	0.00	0.00	0.00	0.00	0.00	1612.85	1612.85
H_2	0.00	0.00	0.00	0.00	0.00	76.00	76.00
NMPI	3674.96	1.84	3673.13	3673.13	3677.93	0.00	3677.93
NMPI-FA Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	3820.16	1.91	3818.25	3823.05	3828.05	0.00	3828.05

Table S11. Operating conditions and mass flow rates of major components in Section 200 of case study B.

Stream	**S-201**	**S-202**	**S-203**	**S-204**	**S-205**	**S-206**	**S-207**	**S-208**	**S-209**	**S-210**
Total Mass Flow (kg/h)	9734.94	9735.03	1384.73	8350.31	568.55	816.18	540.12	28.43	540.12	540.12
Temperature (°C)	120	120	75	75	35	35	93	93	704	120
Pressure (bar)	120.00	120.00	1.01	1.01	1.01	1.01	1.01	1.01	120.01	120.01
Component Mass Flow (kg/h)										
CO_2	1991.17	398.23	398.23	0.00	398.23	0.00	378.32	19.91	378.32	378.32
H_2	133.55	60.58	60.58	0.00	60.58	0.00	57.56	3.03	57.56	57.56
NMPI	3709.80	627.90	120.56	507.34	33.55	87.01	31.87	1.68	31.87	31.87
NMPI-FA Complex	40.07	4787.96	445.87	4342.10	42.18	403.69	40.07	2.11	40.07	40.07
H_2O	3860.35	3860.35	359.48	3500.87	34.01	325.48	32.31	1.70	32.31	32.31

Table S12. Operating conditions and mass flow rates of major components in Section 300 of case study B.

Stream	**S-301**	**S-302**	**S-303**	**S-304**	**S-305**	**S-306**
Total Mass Flow (kg/h)	9166.40	6114.51	15280.90	15280.90	7484.30	7796.60
Temperature (°C)	70.85	80.00	62.97	59.00	28.84	94.10
Pressure (bar)	1.01	1.01	0.20	0.20	0.06	0.06
Component Mass Flow (kg/h)						
Formic Acid	0.00	94.09	94.09	94.09	0.00	94.09
NBI	0.00	5942.48	5942.48	1449.80	0.00	1449.80
NBI-FA Complex	0.00	77.94	77.94	6235.78	0.00	6235.78
NMPI	594.26	0.00	594.26	3674.88	3674.88	0.00
NMPI-FA Complex	4745.79	0.00	4745.79	0.00	0.00	0.00
H_2O	3826.35	0.00	3826.35	3826.35	3809.41	16.94

Table S13. Operating conditions and mass flow rates of major components in Section 300 of case study B.

Stream	S-307	S-308	S-309	S-310	S-311	S-312	S-313
Total Mass Flow (kg/h)	7796.60	7796.60	7796.60	7796.60	1686.66	1686.66	6109.95
Temperature (°C)	96.08	50.29	50.29	95.00	15.62	15.66	135.40
Pressure (bar)	9.06	1.01	0.91	0.91	0.04	1.01	0.04
Component Mass Flow (kg/h)							
Formic Acid	94.09	1759.27	1759.27	1759.27	1665.25	1665.25	94.02
NBI	1449.80	5942.52	5942.52	5942.52	4.47	4.47	5938.05
NBI-FA Complex	6235.78	77.88	77.88	77.88	0.00	0.00	77.88
NMPI	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NMPI-FA Complex	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	16.94	16.94	16.94	16.94	16.94	16.94	0.00

Table S14. Operating conditions and mass flow rates of major components in Section 300 of case study B.

Stream	**S-314**	**S-315**	**S-316**	**S-317**	**S-318**	**S-319**
Total Mass Flow (kg/h)	6109.95	6109.95	6109.95	6109.95	4.56	0.00
Temperature (°C)	129.50	25.00	25.00	25.00	25.00	25.00
Pressure (bar)	1.01	1.01	1.01	1.01	1.01	1.01
Component Mass Flow (kg/h)						
Formic Acid	94.02	94.02	94.02	94.02	0.07	0.00
NBI	5938.05	5938.05	5938.05	5938.05	4.43	0.00
NBI-FA Complex	77.88	77.88	77.88	77.88	0.06	0.00
NMPI	0.00	0.00	0.00	0.00	0.00	0.00
NMPI-FA Complex	0.00	0.00	0.00	0.00	0.00	0.00
H_2O	0.00	0.00	0.00	0.00	0.00	0.00

Table S15. Equipment specification and cost for Case Study A

Main Equipment Quantity/ Standby/ Staggered	Name	Description	Unit Cost ($)	Cost ($)
1 / 0 / 0	V-101	Blending Tank Vessel Volume = 25349.93 L	287,000	287,000
1 / 0 / 0	C-301	Rigorous Distillation Column Column Volume = 4681.40 L	275,000	275,000
1 / 0 / 0	V-103.	Blending Tank Vessel Volume = 19708.98 L	257,000	257,000
1 / 0 / 0	C-401	Rigorous Distillation Column Column Volume = 4967.93 L	252,000	252,000
1 / 0 / 0	PM-101.	Centrifugal Pump Pump Power = 53.15 kW	147,000	147,000
1 / 0 / 0	MSX-101	Mixer-Settler Extractor Rated Throughput = 23232.69 L/h	139,000	139,000
1 / 0 / 0	G-104	Centrifugal Compressor Compressor Power = 81.40 kW	138,000	138,000
1 / 0 / 0	PM-301	Centrifugal Pump Pump Power = 29.41 kW	116,000	116,000
1 / 0 / 0	G-103.	Centrifugal Compressor Compressor Power = 22.39 kW	106,000	106,000
1 / 0 / 0	G-102	Centrifugal Compressor Compressor Power = 48.31 kW	106,000	106,000
1 / 0 / 0	G-101	Centrifugal Compressor Compressor Power = 14.89 kW	106,000	106,000
1 / 0 / 0	PFR-201	Plug Flow Reactor Vessel Volume = 17732.54 L	100,000	100,000

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1 / 0 / 0	PM-103	Centrifugal Pump Pump Power = 19.53 kW	99,000	99,000
1 / 0 / 0	V-301	Decanter Tank Vessel Volume = 636.83 L	69,000	69,000
1 / 0 / 0	PFR-401	Plug Flow Reactor Vessel Volume = 13579.30 L	58,000	58,000
1 / 0 / 0	V-102.	Receiver Tank Vessel Volume = 13.41 L	55,000	55,000
1 / 0 / 0	HX-201	Condenser Condensation Area = 4.58 m2	50,000	50,000
1 / 0 / 0	V-201	Flash Drum Vessel Volume = 2492.47 L	33,000	33,000
1 / 0 / 0	HX-104	Heat Exchanger Heat Exchange Area = 5.30 m2	31,000	31,000
1 / 0 / 0	HX-301	Heat Exchanger Heat Exchange Area = 4.28 m2	27,000	27,000
1 / 0 / 0	HX-302	Heat Exchanger Heat Exchange Area = 2.53 m2	20,000	20,000
1 / 0 / 0	HX-101	Heat Exchanger Heat Exchange Area = 1.90 m2	16,000	16,000
1 / 0 / 0	PM-402	Centrifugal Pump Pump Power = 0.00 kW	13,000	13,000
1 / 0 / 0	PM-401	Centrifugal Pump Pump Power = 0.07 kW	13,000	13,000
1 / 0 / 0	PM-102.	Centrifugal Pump Pump Power = 0.05 kW	13,000	13,000
1 / 0 / 0	HX-102	Heat Exchanger Heat Exchange Area = 0.62 m2	11,000	11,000

SUPPLEMETARY INFORMATION

1 / 0 / 0	HX-105	Heat Exchanger Heat Exchange Area = 0.00 m2	11,000	11,000
1 / 0 / 0	HX-103	Heat Exchanger Heat Exchange Area = 0.47 m2	11,000	11,000
1 / 0 / 0	HX-401	Heat Exchanger Heat Exchange Area = 0.06 m2	11,000	11,000
1 / 0 / 0	GTV-401	Gate Valve Valve Diameter = 0.96 cm	1000	1000
		Unlisted Equipment		643,000
			TOTAL	**3,213,000**

Table S16. Equipment specification and cost for Case Study B

Main Equipment

Quantity/ Standby/ Staggered	Name	Description	Unit Cost ($)	Cost ($)
1 / 0 / 0	C-301	Rigorous Distillation Column Column Volume = 32,602.99 L	2,856,000	2,856,000
1 / 0 / 0	C-302	Rigorous Distillation Column Column Volume = 10,412.24 L	1,738,000	1,738,000
1 / 0 / 0	G-201	Centrifugal Compressor Compressor Power = 351.00 kW	645,000	645,000
1 / 0 / 0	PFR-201	Plug Flow Reactor Vessel Volume = 9281.76 L	473,000	473,000
1 / 0 / 0	PM-107.	Centrifugal Pump Pump Power = 40.49 kW	132,000	132,000
1 / 0 / 0	G-101	Centrifugal Compressor Compressor Power = 20.64 kW	106,000	106,000
1 / 0 / 0	G-103	Centrifugal Compressor Compressor Power = 16.48 kW	106,000	106,000
1 / 0 / 0	G-102.	Centrifugal Compressor Compressor Power = 41.99 kW	106,000	106,000
1 / 0 / 0	V-101.	Blending Tank Vessel Volume = 160.78 L	68,000	68,000
1 / 0 / 0	HX-202	Condenser Condensation Area = 14.38 m2	50,000	50,000
1 / 0 / 0	V-102.	Flat Bottom Tank Vessel Volume = 262.58 L	48,000	48,000
1 / 0 / 0	PM-301	Centrifugal Pump Pump Power = 3.19 kW	44,000	44,000
1 / 0 / 0	HX-201	Heat Exchanger Heat Exchange Area = 4.46 m2	28,000	28,000
1 / 0 / 0	HX-301	Heat Exchanger Heat Exchange Area = 3.72 m2	25,000	25,000

SUPPLEMETARY INFORMATION

1 / 0 / 0	V-201	Flash Drum Vessel Volume = 1445.74 L	24,000	24,000
1 / 0 / 0	HX-203	Heat Exchanger Heat Exchange Area = 2.82 m2	21,000	21,000
1 / 0 / 0	HX-101	Heat Exchanger Heat Exchange Area = 2.44 m2	19,000	19,000
1 / 0 / 0	HX-303	Heat Exchanger Heat Exchange Area = 1.82 m2	16,000	16,000
1 / 0 / 0	PM-303	Centrifugal Pump Pump Power = 0.27 kW	15,000	15,000
1 / 0 / 0	PM-103.	Centrifugal Pump Pump Power = 0.05 kW	13,000	13,000
1 / 0 / 0	PM-101.	Centrifugal Pump Pump Power = 0.03 kW	13,000	13,000
1 / 0 / 0	PM-302	Centrifugal Pump Pump Power = 0.05 kW	13,000	13,000
1 / 0 / 0	HX-302	Heat Exchanger Heat Exchange Area = nan m2	11,000	11,000
1 / 0 / 0	GTV-301.	Gate Valve Valve Diameter = 1.30 cm	1000	1000
		Unlisted Equipment		1.643.000
			TOTAL	**8.213.000**

Table S17. Annual Material Consumption and Cost Summary for Case Study A

Bulk Material	Unit Cost ($)	Annual Amount		Annual Cost ($)	%
Hydrogen	0.70	2,565,309	kg	2,308,779	97.93
Methanol	0.24	198,000	kg	47,520	2.02
Ruthenium(II) h	1,900.00	0	kg	4	0.00
Trihexylamine	20.00	8	kg	317	0.01
Water	3.00	350	MT	1051	0.04
TOTAL				**2,357,670**	**100**

Table S18. Annual Utilities Consumption and Cost Summary for Case Study A

Utility	Unit Cost ($)	Annual Amount	Ref. Units	Annual Cost ($)	%
Std Power	0.10	9,841,225	kW-h	984,123	30.30
Steam	32.00	1,002	MT	32,060	0.99
Cooling Water	0.10	2,186,925	MT	218,693	6.73
Chilled Water	0.50	2,850,120	MT	1,425,060	43.88
Steam MP	35.00	10,778	MT	377,247	11.62
Natural Gas	25.00	8,428	MW-h	210,701	6.49
TOTAL				**3,247,884**	**100**

Table S19. Annual Material Consumption and Cost Summary for Case Study B

Bulk Material	Unit Cost ($)	Annual Amount		Annual Cost ($)	%
Hydrogen	1,50	601.904	kg	902.857	36,58
NBI	25,50	23.344	kg	595.271	24,12

NBI-FA	0,00	294	kg	0	0,00
NMPI	25,50	38.028	kg	969.711	39,29
Water	3,00	78	MT	233	0,01
TOTAL				2.468.072	100,00

Bulk Material	Unit Cost ($)	Annual Amount		Annual Cost ($)	%
Hydrogen	0.7	1289,79	kg	902.857	36.58
NBI	25.50	23,344	kg	595.271	24.12
NBI-FA	0.00	294	kg	0	0.00
NMPI	25.50	38,028	kg	969.711	39.29
Water	3.00	78	MT	233	0.01
TOTAL				**2,468,072**	**100**

Table S20. Annual Utilities Consumption and Cost Summary for Case Study B

Utility	**Unit Cost ($)**	**Annual Amount**	**Ref. Units**	**Annual Cost ($)**	**%**
Std Power	0,10	4.710.860	kW-h	471.086	11,42
Steam	32,00	388	MT	12.429	0,30
Cooling Water	0,10	7.596.660	MT	759.666	18,42
Chilled Water	0,50	812.797	MT	406.398	9,85
Steam MP	35,00	70.694	MT	2.474.276	60,00
TOTAL				4.123.855	100,00

Utility	Unit Cost ($)	Annual Amount	Ref. Units	Annual Cost ($)	%
Std Power	0,10	4,710,860	kW-h	471,086	11.42
Steam	32,00	388	MT	12,429	0.30
Cooling Water	0,10	7,596,660	MT	759,666	18.42
Chilled Water	0,50	812,797	MT	406,398	9.85
Steam MP	35,00	70,694	MT	2,474,276	60.00
TOTAL				**4,123,855**	**100**

Table S21. Economic evaluation parameters for entire project

Time Parameters	Value
Year of analysis	2025
Year Construction starts	2025
Construction Period	30 months
Startup Period	4 months
Project Lifetime	15 years
Inflation	4%

Table S22. Fixed capital estimate summary for Case Study A

Total Plant Direct Cost (TPDC) (physical cost)	
1. Equipment Purchase Cost	3,213,000
2. Installation	1,212,000
3. Process Piping	1,121,000
4. Instrumentation	1,278,000
5. Insulation	96,000
6. Electrical	321,000
7. Buildings	1,436,000
8. Yard Improvement	482,000
9. Auxiliary Facilities	1,278,000
TPDC	10,436,000
Total Plant Indirect Cost (TPIC)	
10. Engineering	2,609,000
11. Construction	3,643,000
TPIC	6,252,000
Total Plant Cost (TPC = TPDC+TPIC)	
TPC	16,688,000
Contractor's Fee & Contingency (CFC)	
12. Contractor's Fee	834,000
13. Contingency	1,669,000
CFC = 12+13	2,503,000
Direct Fixed Capital Cost (DFC = TPC+CFC)	
DFC	19,191,000

Table S23. Fixed capital estimate summary for Case Study B

Total Plant Direct Cost (TPDC) (physical cost)	
1. Equipment Purchase Cost	8,213.000
2. Installation	1,796.000
3. Process Piping	2,875.000
4. Instrumentation	3,285.000
5. Insulation	246,000
6. Electrical	821,000
7. Buildings	3,696,000
8. Yard Improvement	1,232,000
9. Auxiliary Facilities	3,285,000
TPDC	25,450,000
Total Plant Indirect Cost (TPIC)	
10. Engineering	6,362,000
11. Construction	8,907,000
TPIC	15,270,000
Total Plant Cost (TPC = TPDC+TPIC)	
TPC	40,720,000
Contractor's Fee & Contingency (CFC)	
12. Contractor's Fee	2,036,000
13. Contingency	4,072,000
CFC = 12+13	6,108,000
Direct Fixed Capital Cost (DFC = TPC+CFC)	
DFC	46,828,000

Table S24. Annual operating cost for case study A

Cost Item	$	%
Raw Materials	2,358,000	15.36
Labor-Dependent	4,422,000	28.98
Facility-Dependent	4,631,000	30.16
Laboratory/QC/QA	667,000	4.35
Consumables	0	0.00
Waste Treatment/Disposal	0	0.00
Utilities	3,248,000	21.15
Transportation	0	0.00
Miscellaneous	0	0.00
Advertising/Selling	0	0.00
Running Royalties	0	0.00
Failed Product Disposal	0	0.00
TOTAL	15,386,000	100

Table S25. Annual operating cost for case study B

Cost Item	$	%
Raw Materials	2,468,000	13.42
Labor-Dependent	2,166,000	11.78
Facility-Dependent	8.852.000	48.12
Laboratory/QC/QA	325,000	1.77
Consumables	456,000	2.48
Waste Treatment/Disposal	4,000	0.01
Utilities	4,124,000	22.42
Transportation	0	0.00
Miscellaneous	0	0.00
Advertising/Selling	0	0.00

Running Royalties	0	0.00
Failed Product Disposal	0	0.00
TOTAL	18,396,000	100.00