Supporting Information

Biocatalytic Continuous Manufacturing of Diabetes Drug: Plantwide Process Modeling, Optimization, and Environmental and Economic Analysis

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Supporting Information is 12 pages and includes 6 tables (**Table S1, S2 S3 S4 S5** and **S6**) and 2 figure (**Figure S1** and **S2**).

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Table S1. Literature data for the determination of kinetic constant[1]

Time (hr)	Conversion	[A] (g L^{-1})	ln[A]
0	0%	200	5.30
1.5	48%	104	4.64
5	67%	66	4.19
24	89%	22	3.09

Table S2. Implementation steps and parameters of surrogate-based optimization

Implementation step	**1. Initialization**	**2. Fit response surface**	**3. Choose candidate point**	**4. Termination**
	Generate initial points to be evaluated	Approximate the objective function based on evaluated points to build a surrogate model	Generate the candidate points and pick the best one	Stop once criterion met or go back to step 2
Adopted parameters in pySOT	Experimental design : SymmetricLatinHypercube (Symmetric Latin hypercube design)	Surrogate model: RBFInterpolant (Radial basis function)	Adaptive sampling: CandidateDYCORS (Dynamic coordinate search using response surface models)	Evaluation time: 3000 times
Other parameters	• Controller: ThreadController (for parallel computing)		• Strategy: SyncStrategyPenalty (for constrained optimization problem)	
Upper bound & lower bound for decision variables	• Concentration of prositagliptin ketone (mol m^{-3}): [0, 400] • Length of reactor 7 (m): [0, 0.5542] • Flow rate (m^3 hr^{-1}): [0, 0.00039]			

The Experimental design, Surrogate model, Adaptive sampling, Evaluation time, Controller and Strategy are parameters to be tune in pySOT that determine how the optimization is conducted. More details about these parameters can be refer to pySOT documentation.[2]

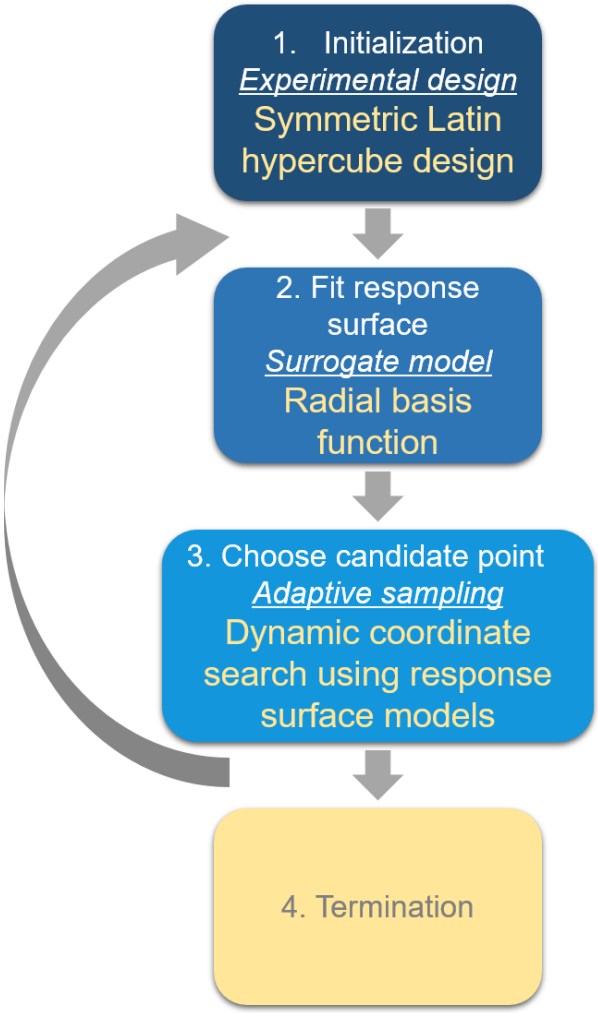

Figure S1. Flowchart of surrogate-based optimization.

Table S3. Summary of the volumetric flow rate and dimensions of all equipment used in biocatalytic continuous sitagliptin manufacturing

	Reactor in Joliffe *et al.*	Reactor 1	Reactor 2	Reactor 3	Reactor 4
Flow rate (mL/hr)	194.08	26.57	208.06	26.53	26.53
Dimension (mL)	78.92	10.80	84.61	10.79	10.79
Reactor 5	Reactor 6	Reactor 7	Reactor 8		Mixer in Joliffe *et al.*
24.67	26.01	130.01	304.2682167	Flow rate (mL/hr)	121.69
10.03	10.58	40	123.726544	Dimension (kW)	0.70
Mixer 1	Mixer 2	Mixer 3	Mixer 4	Mixer 5	Mixer 6
26.57	262.91	208.06	26.53	26.53	255.09
0.15	1.51	1.20	0.15	0.15	1.47
Mixer 7	Mixer 8	Mixer 9	Mixer 10	Mixer 11	Mixer 12
24.67	26.01	78.01	78.70	308.59	46.71
0.14	0.15	0.45	0.45	1.78	0.27
Mixer 13	Mixer 14	Mixer 15	Mixer 16	Mixer 17	Dilution tank 1
276.60	273.26	910.84	459.77	304.27	141.77
1.59	1.57	5.24	2.64	1.75	0.82

Dilution tank 2	Dilution tank 3	Condenser 1	Condenser 2	Condenser 3	Condenser 4
78.01	299.46	224.53	138.89	117.43	218.39
0.45	1.72	1.29	0.80	0.68	1.26
Condenser 5	Condenser 6	Condenser 7	Condenser 8	Wash tank 1	
216.21	413.79	240.81	41.38	12.67427123	Flow rate (mL/hr)
1.24	2.38	1.39	0.24	0.072906483	Dimension
Extraction in Joliffe *et al.*	Extraction 1	Extraction 2	Extraction 3	Extraction 4	Extraction 5
379.58	262.91	308.59	276.60	273.26	910.8434483
5.00	3.46	4.06	3.64	3.60	11.99804321
	Crystallizer in Joliffe *et al.*	Crystallizer 1	Crystallizer 2	Crystallizer 3	Crystallizer 4
Flow rate (mL/hr)	14.39	333.0486097	484.9792564	226.0142894	302.9065788
Dimension (m^3)	0.2	4.628889641	6.740503911	3.141268789	4.2099594
	Filter in Joliffe *et al.*	Filter 1	Filter 2	Filter 3	Filter 4
Flow rate (mL/hr)	77.88	338.3536495	26.53	484.9792564	416.9233803
Dimension (m^2)	0.5	2.172275613	0.170326143	3.11363159	2.676703777
Filter 5	Filter 6		Heat exchanger in Joliffe *et al.*	Heat exchanger 1	Heat exchanger 2
459.7701149	302.9065788	Flow rate (mL/hr)	28.78	26.56985129	26.53
2.951785535	1.944700686	Dimension (m^2)	20	18.46410791	18.43641418
Heat exchanger 3	Heat exchanger 4				
24.66536349	26.01428939				
17.14062786	18.07803293				

Table S4. Estimation of Free-On-Board cost of equipment used in biocatalytic continuous sitagliptin manufacturing

	Reactor		Reactor in Joliffe *et al.*	Reactor 1	Reactor 2
n	1	Dimension (mL)	80.000	26.570	84.605
f	1.0106	Price ($)	147,371	20,556	160,971
Reactor 3	Reactor 4	Reactor 5	Reactor 6	Reactor 7	Reactor 8
10.788	10.788	10.030	10.578	40.000	123.727
20,526	20,526	19,083	20,127	76,105	235,404
	Mixer		Mixer in Joliffe *et al.*	Mixer 1	Mixer 2
n	0.3	Dimension (kW)	5.000	0.153	1.512
f	1.1033	Price ($)	35,269	13,967	27,781
Mixer 3	Mixer 4	Mixer 5	Mixer 6	Mixer 7	Mixer 8
1.197	0.153	0.153	1.467	0.142	0.150
25,898	13,961	13,961	27,530	13,659	13,879
Mixer 9	Mixer 10	Mixer 11	Mixer 12	Mixer 13	Mixer 14
0.449	0.453	1.775	0.269	1.591	1.572
19,295	19,346	29,148	16,544	28,207	28,104
Mixer 15	Mixer 16	Mixer 17	Dilution tank 1	Dilution tank 2	Dilution tank 3
5.239	2.645	1.750	0.816	0.449	1.723
40,331	32,852	29,025	23,082	19,295	28,887
Condenser 1	Condenser 2	Condenser 3	Condenser 4	Condenser 5	Condenser 6

1.292	0.799	0.675	1.256	1.244	2.380
26,496	22,940	21,814	26,277	26,198	31,830
Condenser 7	Condenser 8	Wash tank 1		Extraction	
1.385	0.238	0.073	*n*	0.22	Dimension
27,059	15,953	11,186	*f*	1.1033	Price ($)
Extraction in Joliffe *et al.*	Extraction 1	Extraction 2	Extraction 3	Extraction 4	Extraction 5
10.000	3.463	4.065	3.643	3.599	11.998
27,844	24,863	25,755	25,143	25,075	32,680
	Crystallizer		Crystallizer in Joliffe *et al.*	Crystallizer 1	Crystallizer 2
n	0.68	Dimension (m^3)	75.000	4.629	6.741
f	1.1033	Price ($)	232,034	39,371	50,835
Crystallizer 3	Crystallizer 4		Filter		Filter in Joliffe *et al.*
3.141	4.210	*n*	0.6	Dimension (m^2)	150.000
30,247	36,912	*f*	1.1033	Price ($)	211,336
Filter 1	Filter 2	Filter 3	Filter 4	Filter 5	Filter 6
2.172	0.170	3.114	2.677	2.952	1.945
18,776	4,076	23,304	21,283	22,569	17,570
	Heat exchanger		Heat exchanger in Joliffe *et al.*	Heat exchanger 1	Heat exchanger 2
n	0.71	Dimension (m^2)	100.000	18.464	18.436
f	1.1033	Price ($)	64,969	22,077	22,054
Heat exchanger 3	Heat exchanger 4		Distillation in Joliffe *et al.*	Distillation	Total
17.141	18.078	Amount		6	
20,942	21,749	Price ($)	8,385	8,569	51,415
	Pump in Joliffe *et al.*	Pump	Total		Dryer in Joliffe *et al.*
Amount		60			
Price ($)	1,368	1,398	83,881	Price ($)	31,038
Dryer 1	Ultrafiltration 1				
31,721	600				

The cost estimation of each type of equipment has been calculated based on **Equation 12** and the reference paper.[3] n, f, dimension and price in the cell, for example, "Reactor in Joliffe *et al.*" represents n, f, S_A and $Cost_A$ in **Equation 12**, respectively. This also applies to the other types of equipment. All FOB costs obtained by **Equation 12** are the prices of the year of 2016 by GBP.[3] Thus, the FOB costs obtained by **Equation 12** have been multiplied into an exchange rate of 1.4729 from GBP to USD and a mean inflation rate of 2.2% from January 1st 2017 to July 6th 2018.[4,5] The exchange rate has been sourced from FED on April 4th 2016, the publication date of the reference paper. All FOB costs of the reference paper have also been multiplied into an exchange rate of 1.4279. In the reference paper, all distillation equipment has the same price regardless of the incoming volumetric flow rate; therefore, this has been also considered here. As for the Dryer 1 used in this present paper, since there is limited volumetric flow rate, considering the similar order of magnitude of scale with that of dryer used in reference paper, the same price multiplied into inflation rate and exchange rate has been used.[3] Dilution tank and condenser are simple equipment that are regarded as mixers. Lastly, the price of ultrafiltration membrane has been sourced from vendor.[6]

Table S5. Waste disposal and utility costs used in this present paper

Waste disposal costs in reference	The exchange rate of GBP to USD on April 4th 2016	Mean inflation rate from January 1st 2017 to July 6th 2018	Waste disposal costs in this paper
$ 0.35/L	1.427	1.022	$0.51/L
Utility costs in reference			Utility costs in this paper
$0.95/kg			$1.4/kg

$1.4/kg and $0.51/L come from 1.4279, the exchange rate of GBP to USD on Aril 4 2016 times 1.022 (inflation rate), and times $0.96/kg and $0.35/L respectively, which are used in the publication of Jolliffe *et al*.[3–5]

Table S6. Mass balance across whole process

Mass flow rate (kg/hr)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18 (solid)	18 (solution)	19	20	21
1	0.03409	0.00000	0.03409	0.00341	0.00000	0.00000	0.00341	0.00068	0.00273	0.00000	0.00273	0.00273	0.00000	0.00273	0.00273	0.00000	0.00000	0.00000	0.00273	0.00000	0.00273	0.00000
H_2O	0.00000	0.02657	0.02657	0.02657	0.00000	0.00000	0.02657	0.02657	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NH_2NH_2	0.00000	0.01431	0.01431	0.00572	0.00000	0.00000	0.00572	0.00572	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.02950	0.00000	0.00000	0.02950	0.00361	0.02589	0.00000	0.02589	0.02589	0.00000	0.02589	0.00777	0.00000	0.00000	0.00000	0.00777	0.00000	0.00777	0.00000
HCl	0.00000	0.00000	0.00000	0.00977	0.00000	0.00000	0.00977	0.00977	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2-propanol	0.00000	0.00000	0.00000	0.00000	0.00147	0.02950	0.02950	0.00000	0.02950	0.02802	0.00147	0.01353	0.00000	0.01353	0.01353	0.00000	0.00000	0.00000	0.01353	0.00000	0.01353	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.01327	0.26548	0.26548	0.00000	0.26548	0.25220	0.01327	0.01327	0.00000	0.01327	0.01327	0.00000	0.00000	0.00000	0.01327	0.00000	0.01327	0.00000
IPAc	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.00000	0.10000	0.10000	0.00000	0.00000	0.00000	0.10000	0.00000	0.10000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.09877	0.09877	0.02963	0.00000	0.00000	0.00000	0.02963	0.00000	0.02963	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.04973	0.00000	0.00000	0.03481	0.01492	0.00000	0.01492	0.00000
Trifluoroacetic acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.03753	0.00000	0.00000	0.00000	0.03753	0.00000	0.03753	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.00500	0.00000	0.00000	0.00000	0.00000	0.09500
Superphosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01000	0.01000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
i-$PrNH_2$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Phosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Mass flow rate (kg/hr)	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37 (Pd catalyst)	38	39	40	41	42	43
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00273	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2O	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.22857	0.00000	0.00000	0.00000	0.22857
NH_2NH_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00777	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.09698	0.00000	0.00000	0.00000	0.10000
2-propanol	0.01218	0.00012	0.01206	0.00000	0.01206	0.00135	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.01327	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPAc	0.09000	0.00090	0.08910	0.01090	0.10000	0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.02963	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.01492	0.03481	0.00000	0.03481	0.00348	0.00348	0.00000	0.00000	0.00000	0.00348	0.00000	0.00348	0.00348	0.00000	0.00000	0.00000	0.00000
Trifluoroacetic acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.03753	0.00000	0.00000	0.00000	0.01182	0.01182	0.00000	0.00000	0.00000	0.01182	0.00000	0.01182	0.01182	0.00000	0.00000	0.00000	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00500	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Superphosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.01000	0.00000	0.05000	0.05000	0.05000	0.05000	0.00000	0.00000	0.00000	0.05000	0.00000	0.05000	0.05000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01951	0.01951	0.00000	0.00000	0.00000	0.00390	0.00000	0.00390	0.00390	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01000	0.00967	0.00033	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01577	0.00000	0.01577	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01880	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20000	0.01000	0.19000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
i-$PrNH_2$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Phosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Mass flow rate (kg/hr)	44 (solid)	44 (solution)	45	46	47	48	49	50	51	52	53	54	55	56	57	58 (solid)	58 (solution)	59	60	61	62	63
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2O	0.00000	0.22857	0.22857	0.00000	0.22857	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20000	0.00000	0.20000	0.30000	0.00000	0.10000	0.04086	0.04086
NH_2NH_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCl	0.00000	0.09698	0.09698	0.00000	0.09698	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00214	0.00000	0.00000	0.00214	0.00214	0.00000	0.00000	0.00000	0.00000
2-propanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPAc	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00348	0.00348	0.00000	0.00348	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Trifluoroacetic acid	0.00000	0.01182	0.01182	0.00000	0.01182	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Superphosphoric acid	0.00000	0.05000	0.05000	0.00000	0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00390	0.00390	0.00000	0.00390	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.01331	0.00548	0.00548	0.01331	0.00548	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01331	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.20000	0.20000	0.00000	0.01000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.01176	0.00000	0.00000	0.00000	0.01176	0.00035	0.00000	0.00035	0.00035	0.00000	0.00000	0.00035	0.00035	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00891	0.00000	0.00000	0.00891	0.00045	0.00000	0.00045	0.00045	0.00000	0.00000	0.00045	0.00045	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00746	0.00000	0.00746	0.00746	0.00000	0.00746	0.00746	0.00000	0.00000	0.00746	0.00746	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01483	0.01483	0.01483	0.00000	0.01483	0.01483	0.00000	0.00000	0.01483	0.01483	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.01858	0.00000	0.01858	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00129	0.00000	0.00129	0.00129	0.00000	0.00000	0.00129	0.00129	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00201	0.00201	0.00201	0.00000	0.00000	0.00201	0.00201	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.02387	0.00000	0.02111	0.00276	0.00276	0.02111	0.00000	0.00000	0.02111
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00588	0.00000	0.00000	0.00588	0.00588	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.00000	0.10000	0.04086	0.04086
i-$PrNH_2$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Phosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Mass flow rate (kg/hr)	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2O	0.00000	0.04086	0.02724	0.06810	0.06810	0.04086	0.00070	0.04156	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.04156	0.04156	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NH_2NH_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00030	0.00030	0.00000	0.00000	0.00000	0.00000	0.00000	0.00027	0.00003	0.00030	0.00027	0.00000	0.00000	0.00000	0.00000	0.00000
2-propanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPAc	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20000	0.01190	0.18810	0.00190	0.19000	0.20000	0.00000	0.20000	0.01000	0.00400	0.36000	0.36400	0.20000	0.16400
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Trifluoroacetic acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Superphosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.02111	0.00001	0.02112	0.00003	0.00002	0.00000	0.00002	0.00000	0.00000	0.00000	0.00000	0.00000	0.00002	0.00000	0.00002	0.00002	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.04086	0.02724	0.06810	0.06810	0.04086	0.00000	0.04086	0.00000	0.00000	0.00000	0.00000	0.00000	0.03677	0.00409	0.04086	0.03677	0.00000	0.00000	0.00000	0.00000	0.00000
i-$PrNH_2$	0.03074	0.03074	0.01943	0.05017	0.04857	0.02914	0.00000	0.02914	0.00000	0.00000	0.16065	0.00162	0.16227	0.17081	0.01898	0.18979	0.00854	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00734	0.00734	0.01834	0.01101	0.00000	0.01101	0.00000	0.00000	0.00000	0.00000	0.00000	0.00099	0.01002	0.01101	0.00099	0.00000	0.00000	0.00000	0.00000	0.00000
Acetone	0.00000	0.00000	0.00105	0.00105	0.00262	0.00157	0.00000	0.00157	0.00000	0.00000	0.00000	0.00000	0.00000	0.00141	0.00016	0.00157	0.00141	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00405	0.00405	0.01011	0.00607	0.00000	0.00607	0.00000	0.00000	0.00000	0.00000	0.00000	0.00607	0.00000	0.00607	0.00607	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Phosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Mass flow rate (kg/hr)	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104 (anhydrous Na_2SO_4)	105	106	107
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2O	0.00000	0.00000	0.00144	0.04300	0.04300	0.00000	0.04300	0.04300	0.04300	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NH_2NH_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2-propanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPAc	0.20000	0.03600	0.00000	0.00000	0.20000	0.20000	0.00000	0.20000	0.00000	0.20000	0.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.40000	0.40000	0.00000	0.40000	0.04000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Trifluoroacetic acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Superphosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.00000	0.00000	0.00409	0.00409	0.00368	0.00041	0.00041	0.00004	0.00037	0.40451	0.40451	0.00405	0.40047	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
i-$PrNH_2$	0.00000	0.00000	0.00000	0.01898	0.01898	0.01708	0.00190	0.00190	0.00019	0.00171	1.87895	1.87895	0.01879	1.86016	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00000	0.01002	0.01002	0.00781	0.00220	0.00220	0.00013	0.00207	0.01097	0.00110	0.00001	0.00109	0.00000	0.00000	0.00987	0.00987	0.00000	0.00987	0.00987	0.00000
Acetone	0.00000	0.00000	0.00000	0.00016	0.00016	0.00014	0.00002	0.00002	0.00000	0.00001	0.01554	0.01554	0.00016	0.01538	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00056	0.00054	0.00054	0.00048	0.00005	0.00005	0.00001	0.00005	0.05303	0.05303	0.00053	0.05250	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00005	0.00005	0.00004	0.00000	0.00000	0.00000	0.00000	0.00483	0.00483	0.00005	0.00478	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.10000	0.10000	0.00100	0.09900	0.00100	0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.20000
Phosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

Mass flow rate (kg/hr)	108	109	110	111	112	113	114 (solid)	114 (solution)	115	116	117	118	119	120	121	122	123
1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2O	0.00000	0.00000	0.00000	0.00126	0.00126	0.00126	0.00000	0.00126	0.00126	0.00126	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NH_2NH_2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
HCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2-propanol	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
dichloromethane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPAc	0.00000	0.00000	0.04000	0.00000	0.04000	0.04000	0.00000	0.04000	0.04000	0.00400	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
4	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Trifluoroacetic acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
heptane	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Superphosphoric acid	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
H_2 gas	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
9	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
PivCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
IPEA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
10	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R5	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
TFA	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
11	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R6	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
DMSO	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
i-$PrNH_2$	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
12	0.00000	0.00000	0.00987	0.00000	0.00987	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Acetone	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
by-product from R7	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaOH	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
NaCl	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Brine	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
Ethanol	0.01000	0.19000	0.20000	0.00000	0.20000	0.20000	0.00000	0.20000	0.20000	0.01000	0.00000	0.00000	0.00010	0.01000	0.00010	0.00990	0.01000
Phosphoric acid	0.00000	0.00000	0.00000	0.00713	0.00713	0.00475	0.00000	0.00475	0.00475	0.00475	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
13	0.00000	0.00000	0.00000	0.00000	0.00000	0.01225	0.01102	0.00122	0.00122	0.00122	0.01102	0.01102	0.00000	0.00000	0.00000	0.00000	0.00000

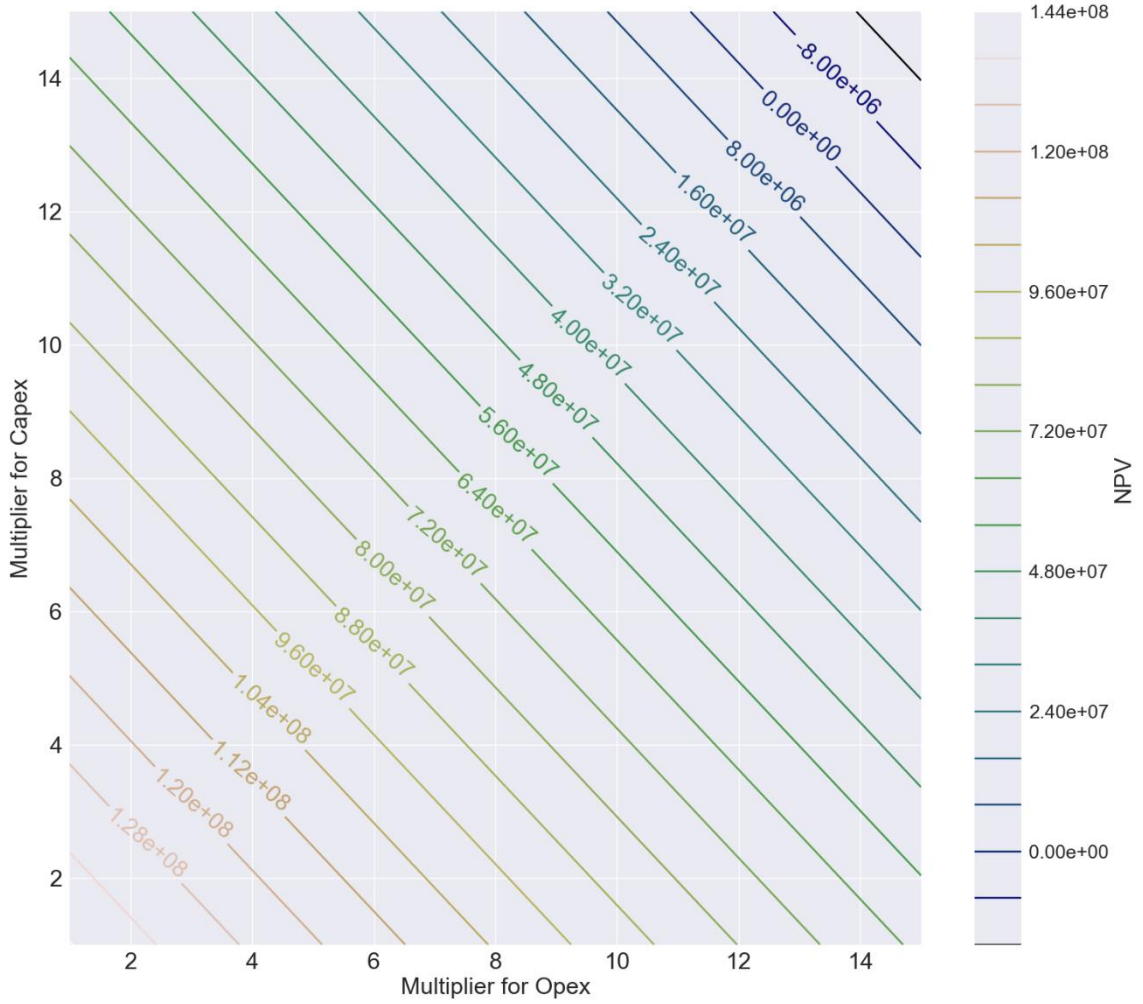

Figure S2. Sensitivity analysis on uncovered costs. To consider the effect of uncovered costs to NPV, current Opex and Capex have been multiplied into multiplier ranging from 1 to 15.

Reference:

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