

Supplement

Prospective Evaluation of Spent Sulfuric Acid Recovery by Process Simulation

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Table S1 Stream results regarding to the simulation of the azeotropic distillation process.

Parameters	Units	ACID-IN	F-WATER	ACID1	CYCLO-2	DISTIL	MAKEUP	D-WATER	ACID-OUT
Phase		L	V	L	L	V	L	L	L
Temperature	°C	25	119	119	60	73	40	60	203
Pressure	bar	1.00	0.93	0.93	1.20	1.10	1.10	1.20	1.30
Mass density	kg/m ³	1147.6	0.5	1218.0	741.9	2.5	760.6	983.2	1360.7
Average MW		22	18	26	84	63	84	18	40
Mass flows									
Total	kg/h	40000	18344	21656	97534	107263	0	9729	11927
Sulfuric acid	kg/h	8000	0	8000	0	0	0	0	8000
Water	kg/h	32000	18344	13656	70	9798	0	9729	3927
Cyclohexane	kg/h	0	0	0	97464	97464	0	0	0
Mass fractions									
Sulfuric acid		20 %	0 %	37 %	0 %	0 %	0 %	0 %	67 %
Water		80 %	100 %	63 %	0 %	9 %	0 %	100 %	33 %
Cyclohexane		0 %	0 %	0 %	100 %	91 %	100 %	0 %	0 %

Table S2 Stream results regarding to the simulation of the counter-current evaporation process.

Parameters	Units	ACID-IN	ACID1	ACID2	STEAM	V-1	V-2	V-3	VAP-OUT	ACID-OUT
Phase		L	L	L	V	V	V	V	L	L
Temperature	°C	25	77	112	198	77	112	197	463	197
Pressure	bar	1.00	0.30	0.80	15.00	0.30	0.80	1.00	1.00	1.00
Mass density	kg/m ³	1147.6	1158.9	1210.1	7.3	0.2	0.5	0.5	989.9	1379.8
Average MW		22	22	25	18	18	18	18	18	40
Mass flows										
Total	kg/h	40000	32767	22852	16340	7233	9916	11090	7233	11761
Sulfuric acid	kg/h	8000	8000	8000	8000	0	0	2	0	7998
Water	kg/h	32000	24767	14852	16340	7233	9916	11088	7233	3764
Mass fractions										
Sulfuric acid		20 %	24 %	35 %	0 %	0 %	0 %	0 %	0 %	68 %
Water		80 %	76 %	65 %	100 %	100 %	100 %	100 %	100 %	32 %

