Supplementary Materials

S1. Data from the Designs Studied

This work is based on the hybrid schemes to purify LA reported by Alcocer-García et al. [1], and Alcocer-García et al. [2]. Tables S1-S5 show the design parameters for the study schemes.

Table S1. Design parameters for conventional schemes.

	Parameter	CS1 [1]	CS2 [2]	CS3 [2]
C1	Number of stages	22	24	28
	Extractant (t/h)	106.722	106.154	106.018
	Diameter (m)	1.434	0.538	0.987
C2	Number of stages	28	24	17
	Feed stage	13	16	11
	Reflux (kg/kg)	0.076	0.025	0.026
	Reboiler duty (MW)	23.026	10.278	9.403
	Diameter (m)	3.642	0.653	1.276
C3	Number of stages	46	39	35
	Feed stage	34	32	9
	Reflux (kg/kg)	0.206	64.901	0.125
	Reboiler duty (MW)	4.465	3.311	13.935
	Diameter (m)	2.413	0.431	0.983
C4	Number of stages	60	39	56
	Feed stage	28	13	16
	Reflux (kg/kg)	54.199	0.11	43.9
	Reboiler duty (MW)	3.486	13.571	3.237
	Diameter (m)	2	0.512	1.662
Levulinic acid (%w/w)		0.98	0.98	0.981
Formic acid (%w/w)		0.851	0.85	0.857
Furfural (%w/w)		0.999	0.999	0.999
TAC ($/y)		1.85E+07	1.56E+07	1.49E+07
EI99 (points/y)		5.36E+09	4.70E+09	4.60E+09

Table S2. Design parameters for thermally coupled schemes.

	Parameter	TCS1 [2]	TCS2 [2]	TCS3 [2]
C1	Number of stages	29	28	27
	Extractant (t/h)	106.061	106.064	106.015
	Diameter (m)	0.633	1.289	0.544
C2	Number of stages	17	17	23
	Feed stage	4,17	10	14,23
	Reflux (kg/kg)	-	0.034	-
	Reboiler duty (MW)	0	9.427	0
	Diameter (m)	1.389	0.758	0.832
C3	Number of stages	31	34	33
	Feed stage	12	15,1	13,1

	Reflux (kg/kg)	0.116	-	-
	Reboiler duty (MW)	23.169	14.077	28.712
	Diameter (m)	0.578	1.230	1.522
	Steam outlet stage	13	-	14
	Steam flow (kg/h)	75669.886	-	78029.651
C4	Number of stages	58	23	25
	Feed stage	32	21	23
	Reflux (kg/kg)	43.139	247.23	337.03
	Reboiler duty (MW)	3.2	0.848	1.138
	Diameter (m)	1.547	1.653	1.751
	Liquid outlet stage	-	20	22
	Liquid flow (kg/h)	-	14336.512	59254.342
Levulinic acid (%w/w)		0.981	0.983	0.986
Formic acid (%w/w)		0.855	0.853	0.862
Furfural (%w/w)		0.999	0.999	1
TAC ($/y)		1.64E+07	1.39E+07	1.90E+07
EI99 (points/y)		4.56E+09	4.21E+09	5.16E+09

Table S3. Design parameters for Intensified schemes studied: TES1, DWCS1, and SI1.

	Parameter	**TES1 [2]**	**DWCS1 [2]**	**SI1 [2]**
C1	Number of stages	27	27	26
	Extractant (t/h)	106.031	106.031	106.024
	Diameter (m)	1.164	0.987	1.359
C2	Number of stages	24	24	19
	Feed stage	15	14	14
	Reflux (kg/kg)	0.041	0.031	0.402
	Reboiler duty (MW)	9.436	9.417	9.442
	Diameter (m)	1.138	1.324	0.836
C3	Number of stages	41	41	49
	Feed stage	26,15	26,15	18
	Reflux (kg/kg)	239.790	239.805	353.25
	Reboiler duty (MW)	14.230	14.25	20.722
	Diameter (m)	1.488	0.678	1.139
	Steam outlet stage	16	16	-
	Steam flow (kg/h)	100591.162	100593.475	-
	Side outlet			14
	Side outlet flow (kg/h)			100505.101
C4	Number of stages	8	9	-
	Feed stage	2	2	-
	Reboiler duty (MW)	1.41	1.41	-
	Diameter (m)	1.031	0.662	-
	Liquid outlet stage	1	1	-
	Liquid flow (kg/h)	110210.787	110210.788	-
Levulinic acid (%w/w)		0.981	0.981	0.981
Formic acid (%w/w)		0.851	0.857	0.857

Furfural (%w/w)	0.999	0.999	0.999
TAC ($/y)	1.43E+07	1.43E+07	1.77E+07
EI99 (points/y)	4.35E+09	4.34E+09	5.22E+09

Table S4. Design parameters for Intensified schemes studied: DWCS-D, DWCS-DA, and TDWS-D.

	Parameter	**DWCS-D [1]**	**DWCS-DA [1]**	**TWCS-D [1]**
C1	Number of stages	21	25	24
	Extractant (t/h)	107.975	106.610	107.752
	Diameter (m)	0.529	1.054	0.634
C2	Number of stages	28	25	16
	Feed stage	11	6	15
	Reflux (kg/kg)	0.069	-	-
	Reboiler duty (MW)	23.188	-	-
	Diameter (m)	3.577	1.437	0.573
C3	Number of stages	20	46	20
	Feed stage	4	25	16
	Steam outlet stage	-	26	17
	Steam flow (t/h)	-	45.756	69.032
	Diameter (m)	1.664	3.04	1.301
C4	Number of stages	62	29	25
	Feed stage	20	14	3
	Feed stage 2			23
	Reflux (kg/kg)	8.205	0.253	345.046
	Reboiler duty (MW)	4.740	26.478	27.215
	Liquid flow (t/h)			773.515
	Steam flow (t/h)	30.024	61.448	102.447
	Liquid outlet stage			2
	Steam outlet stage	21	15	8
	Liquid outlet stage			20
	Diameter (m)	1.984	1.766	2.259
Levulinic acid (%w/w)		0.98	1	0.986
Formic acid (%w/w)		0.953	0.912	0.859
Furfural (%w/w)		0.999	0.999	0.999
TAC ($/y)		1.71E+07	1.69E+07	2.05E+07
EI99 (points/y)		4.83E+09	5.58E+09	5.58E+09

Table S5. Energy requirements and the amount of LA produced.

Scheme	**Reboiler duty (MW)**	**Condenser duty (MW)**	**LA Production kg/year**
CS1	30.977	-23.352	5.28E+07
CS2	27.160	-19.921	5.32E+07
CS4	26.575	-18.988	5.30E+07
TCS1	26.369	-18.853	5.33E+07
TCS2	24.352	-17.427	5.33E+07
TCS3	29.850	-22.721	5.34E+07
TES1	24.986	-17.580	5.34E+07

DWCS1	25.077	-17.510	5.34E+07
SI1	30.164	-22.845	5.34E+07
DWCS-D	27.929	-20.490	5.27E+07
TDWS-D	32.253	-2.870	5.26E+07
DWCS-DA	26.478	-35.204	5.19E+07

References

1. Alcocer-García, H.; Segovia-Hernández, J.G.; Prado-Rubio, O.A.; Sánchez-Ramírez, E.; Quiroz-Ramírez, J.J. Multi-objective optimization of intensified processes for the purification of levulinic acid involving economic and environmental objectives. *Chem. Eng. Process. Process Intensif.* **2019**, *136*, 123–137. https://doi.org/10.1016/j.cep.2019.01.008.
2. Alcocer-García, H.; Segovia-Hernández, J.G.; Sánchez-Ramírez, E.; Caceres-Barrera, C.R.; Hernández, S. Sequential synthesis methodology in the design and optimization of sustainable distillation sequences for levulinic acid purification. *Bioenergy Res.* **2024**, *17*, 1724–1738. https://doi.org/10.1007/s12155-024-10765-0.