

Are deep eutectic solvents really green?: A life-cycle perspective

Electronic Supplementary Information

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Table S1: Ecoinvent unit processes for the foreground processes for choline chloride/urea (reline) deep eutectic solvent (DES) production.

#	Flow	Ecoinvent unit process
1	Ethylene oxide (EO)	market for ethylene oxide ethylene oxide APOS, S - RoW
2	Hydrochloric acid (HCl)	market for hydrochloric acid, without water, in 30% solution state hydrochloric acid, without water, in 30% solution state APOS, S - RoW
3	Trimethylamine (TMA)	market for trimethylamine trimethylamine APOS, S - RoW
4	Deionized water (DI)	market for water, deionised water, deionised APOS, S - RoW
5	Heat (steam)	steam production, as energy carrier, in chemical industry heat, from steam, in chemical industry APOS, S - RoW
6	Electricity	electricity, high voltage, production mix electricity, high voltage APOS, S
7	Urea	market for urea urea APOS, S - RoW
8	Methanol	methanol production methanol APOS, S
9	Ethanol	market for ethanol, without water, in 99.7% solution state, from ethylene ethanol, without water, in 99.7% solution state, from ethylene APOS, S - RoW
10	Dichloromethane (DCM)	dichloromethane production dichloromethane APOS, S
11	Ethyl acetate	ethyl acetate production ethyl acetate APOS, S
12	Ethylene glycol (EG)	market for ethylene glycol ethylene glycol APOS, S
13	Glycerol (Gly)	market for glycerine glycerine APOS, S - RoW
14	Citric acid (CA)	market for citric acid citric acid APOS, S - GLO
15	Glucose (Glu)	market for glucose glucose APOS, S - GLO

Table S2: Calculations of auxiliary processes for choline chloride and reline production

				Ton	kg
MIXER	Q		J	MJ	KWh
			129600	0.13	3.60E-02
	ρ	kg/m ³	1000		3.60E-05
	t	s	7200		
REACTOR 1 (ChCl)	Q		J	MJ	KWh
			3.58E+08	358.46	9.96E+01
	Cp	J/(kg*K)	4181		9.96E-02
	m	kg	1428		
	T(reaction)	K	343		
	t	s	7200		
	η (heat)		0.75		
EVAPORATOR	Q		J	MJ	
			3.06E+09	3.06E+03	3.056722
	Cp	J/(kg*K)	4181		
	m	kg	1428		
	T(boil)	K	373.15		
	To	K	298.15		
	ΔH (vap)	J/kg	2256453		
	m (vap)	kg	885.28		
	η (dry)		0.8		
GRINDER (urea)	Q		J	MJ	KWh
			20053500	20.05	5.57E+00
	m	kg	461		5.57E-03
PRE-MIXER (ChCl+urea)	Q		J	MJ	KWh
			11404.8	0.01	3.17E-03
	ρ	kg/m ³	1320		3.17E-06
	t	s	480		
REACTOR 2 (Reline)	Q		J	MJ	KWh
			2.68E+08	267.68	7.44E+01
	Cp	J/(kg*K)	4181		7.44E-02
	m	kg	1200		
	Tr	K	338.15		
	t	s	540		
	η (heat)		0.75		

Table S3 Environmental Impacts of the reline production process

Impact category	Unit	EO	HCl	TMA	DI	Heat	Electricity
GWP	kg CO ₂ -Eq	1.78E+02	1.40E+02	2.66E+02	6.32E-02	3.66E+02	7.14E+01
FEP	kg P-Eq	4.15E-02	6.77E-02	5.02E-02	2.62E-05	4.37E-02	5.78E-04
TAP	kg SO ₂ -Eq	5.43E-01	7.53E-01	9.15E-01	4.01E-04	1.07E+00	1.29E-01
MDP	kg Fe-Eq	4.68E+00	1.63E+01	1.17E+01	8.75E-03	1.75E+00	3.44E-01
WDP	m ³	3.33E-01	6.06E-01	6.55E-01	1.53E-01	6.76E-01	9.80E-03
FETP	kg 1,4-DCB-Eq	2.58E+00	7.81E+00	5.61E+00	3.88E-03	1.88E+00	2.88E-01
HTP	kg 1,4-DCB-Eq	3.37E+01	9.85E+01	5.60E+01	3.09E-02	5.34E+01	2.49E+00

Impact category	Unit	ChCl	Electricity	Urea	Reline (per ton)	Reline (per kg)
GWP	kg CO ₂ -Eq	1.02E+03	3.22E+01	7.67E+02	1.82E+03	1.82E+00
FEP	kg P-Eq	2.04E-01	3.46E-02	2.33E-01	4.71E-01	4.71E-04
TAP	kg SO ₂ -Eq	3.41E+00	5.87E-02	3.41E+00	6.88E+00	6.88E-03
MDP	kg Fe-Eq	3.47E+01	2.99E-01	5.19E+01	8.70E+01	8.70E-02
WDP	m ³	2.43E+00	1.73E-01	2.18E+00	4.78E+00	4.78E-03
FETP	kg 1,4-DCB-Eq	1.82E+01	6.67E-01	2.19E+01	4.07E+01	4.07E-02
HTP	kg 1,4-DCB-Eq	2.44E+02	2.19E+01	2.51E+02	5.17E+02	5.17E-01

Table S4 Environmental Impacts of the reline and conventional organic solvents (1.0 kg reline, 1.0 kg methanol, 1.0 kg ethanol, 2.4 kg DCM, and 1.2 kg ethyl acetate)

Indicator	Unit	Reline	Methanol	Ethanol	DCM	Ethyl acetate
GWP	kg CO ₂ -Eq	1.82E+00	5.90E-01	9.67E-01	8.23E+00	3.60E+00
FEP	kg P-Eq	4.71E-04	5.79E-05	1.80E-04	1.62E-04	1.45E-03
TAP	kg SO ₂ -Eq	6.88E-03	1.74E-03	1.39E-02	5.01E-02	1.56E-02
MDP	kg Fe-Eq	8.70E-02	1.18E-02	2.29E-02	5.39E-03	1.45E-01
WDP	m ³	4.78E-03	4.29E-03	1.03E-02	2.51E-02	5.10E-02
FETP	kg 1,4-DCB-Eq	4.07E-02	1.04E-02	2.37E-02	9.52E-03	9.30E-02
HTP	kg 1,4-DCB-Eq	5.17E-01	8.58E-02	1.40E-01	1.31E+00	1.10E+00

Table S5 Toxicity (LD₅₀ based on oral-rat) of conventional solvents and the constituents of DESs.

All the values are obtained from RSC ChemSpider database.

Chemical (Solvent)	LD ₅₀ (mg/kg)	Chemical (DES constituent)	LD ₅₀ (mg/kg)
Methanol	5,628	Choline Chloride	3,400
Ethanol	7,060	Urea	8,471
DCM	1,600	Ethylene glycol	4,700
Ethyl acetate	5,620	Glycerol	8,700
		Citric acid	11,700
		Glucose	25,800

Table S6 Environmental Impacts of the reline and other choline chloride-based DESs including NADES (1 kg each).

Indicator	Unit	Reline	ChCl:EG	ChCl:Gly	ChCl:CA	ChCl:Glu
GWP	kg CO ₂ -Eq	1.82E+00	2.00E+00	2.55E+00	4.30E+00	1.61E+00
FEP	kg P-Eq	4.71E-04	4.39E-04	4.90E-04	1.29E-03	4.26E-04
TAP	kg SO ₂ -Eq	6.88E-03	6.51E-03	9.84E-03	2.58E-02	1.02E-02
MDP	kg Fe-Eq	8.70E-02	7.51E-02	7.41E-02	2.43E-01	1.01E-01
WDP	m ³	5.00E-03	4.61E-03	3.51E-02	2.00E-01	9.45E-03
FETP	kg 1,4-DCB-Eq	4.07E-02	3.83E-02	4.77E-02	1.29E-01	5.04E-02
HTP	kg 1,4-DCB-Eq	5.17E-01	4.69E-01	4.38E-01	1.51E+00	4.44E-01