Supplementary Materials

On the Viscosity and Pipe Transport Behavior of Pure Ionic Liquids and Their Mixtures with Conventional Solvents

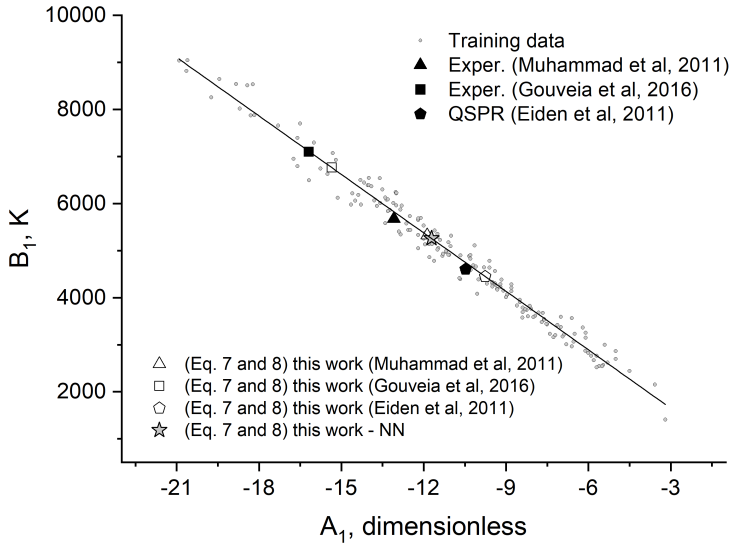


Figure S1. Experimental and fitted values of the A_1 and B_1 parameters in Andrade's equation for the [emim][Ser] IL. For comparison purposes, the data used in the regression of Equations (1), (7), and (8) are presented [11,34,35].

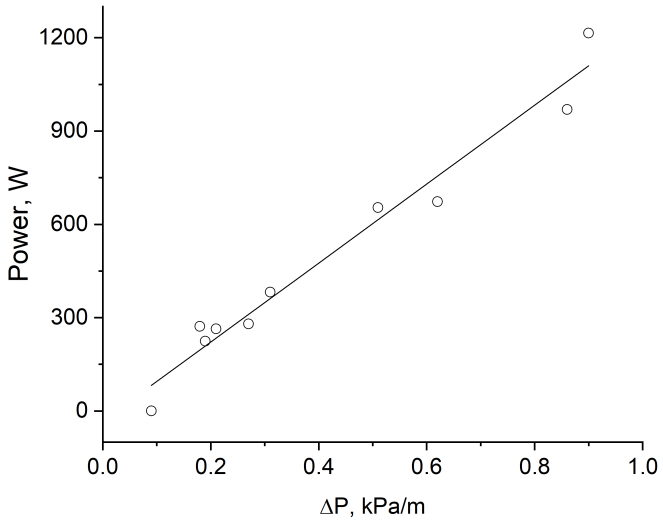


Figure S2. Correlation between the pumping power required to move the fluid and the pressure drop in the pipe. Transport conditions and numerical results are provided in Table 6.

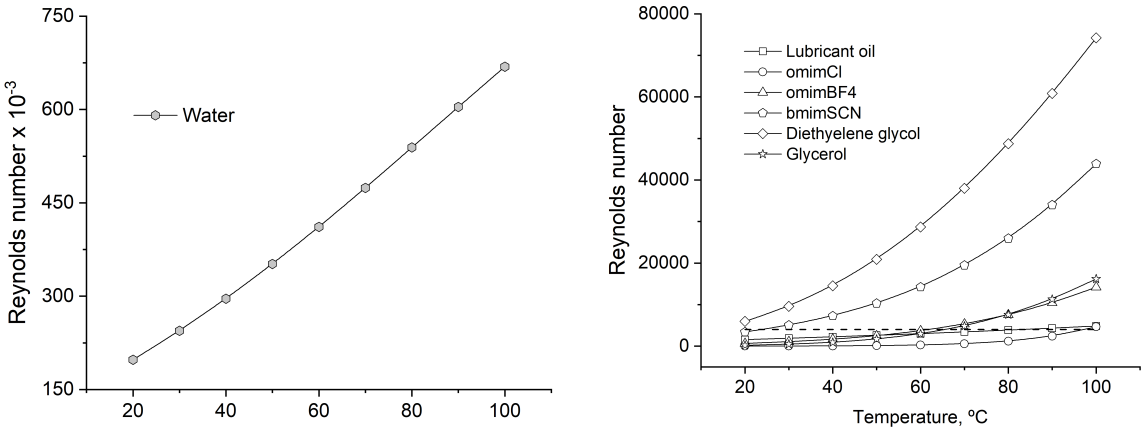
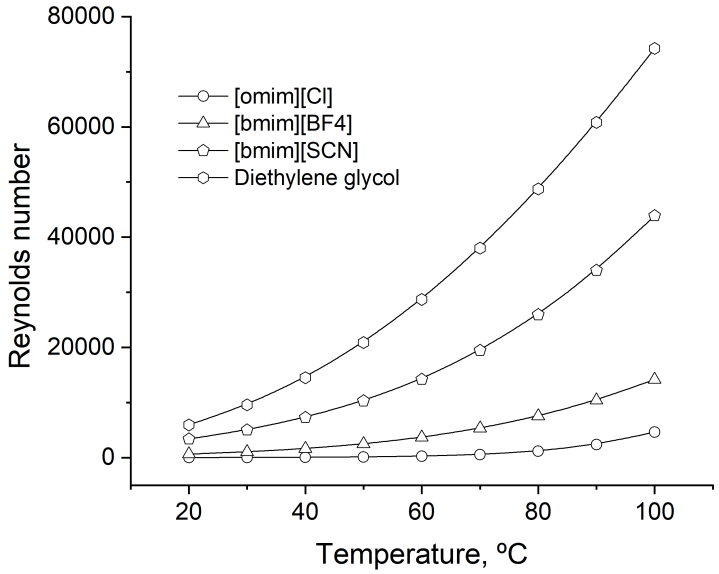


Figure S3. Dependence of the Reynolds number on temperature for selected ILs and conventional solvents. Inner pipe diameter: 203.2 mm; fluid velocity: 1.0 m/s. The horizontal dashed line corresponds to Re = 4000.



$Re = A \cdot exp\left[B \cdot \left({}^{T}/_{\circ C}\right)\right]$		
Fluid	A	B
[omim][Cl]	1.584	0.0820
[bmim][BF_4]	337.4	0.0385
[bmim][SCN]	1970	0.0319
Diethylene glycol	3901	0.0311
Water	157617	0.0151

Figure S4. Exponential dependence of the Reynolds number on temperature for various ILs and conventional solvents. Inner pipe diameter: 203.2 mm; fluid velocity: 1.0 m/s. All regressions yielded $R^2 > 0.99$.

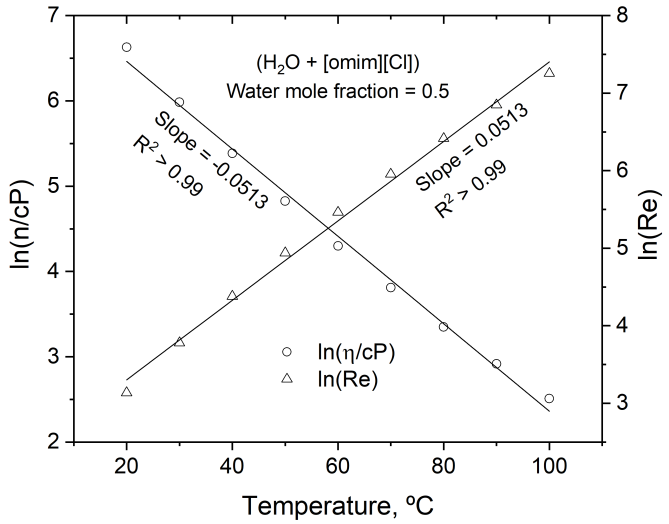


Figure S5. Temperature dependence of ln(η/cP) and ln(Re) for an equimolar (H_2O + [omim][Cl]) mixture. Operating conditions: mixture mass flow rate = 10 t/h, internal pipe diameter = 203.2 mm, pipe length = 1 m, adiabatic transport. Similar behavior was observed for (H_2O + [omim][Cl]) and (MeOH + [omim][Cl]) mixtures with molar fractions of the conventional solvent varying from 0 to 1.

Table S1. Doehlert design matrix for the study of influence of the transport conditions on the pressure drop for pure ILs and conventional solvents (first computational experiment described in Computational Details).

	Exp.	Real Variables				Coded Variables			
	No.	T. °C	D. mm	v. m/s	IL nature	X1	X2	X3	X4
			304.8	1.50			0.866	0.816	
			279.4	1.33			0.577	0.612	
		100	254.0	1.17		1.0	0.289	0.204	
Levels		80	228.6	1.00		0.5	0	0	
		60	203.2	0.83	IL3	0	−0.289	−0.204	0.791
		40	177.8	0.67	IL2	−0.5	−0.577	−0.612	0
		20	152.4	0.50	IL1	−1.0	−0.866	−0.816	−0.791
	1	60	228.6	1.00	IL2	0	0	0	0
	2	100	228.6	1.00	IL2	1.0	0	0	0
	3	20	228.6	1.00	IL2	−1.0	0	0	0
	4	80	304.8	1.00	IL2	0.5	0.866	0	0
	5	40	304.8	1.00	IL2	−0.5	0.866	0	0
	6	80	152.4	1.00	IL2	0.5	−0.866	0	0
	7	40	152.4	1.00	IL2	−0.5	−0.866	0	0
	8	80	254.0	1.50	IL2	0.5	0.289	0.816	0
	9	40	254.0	1.50	IL2	−0.5	0.289	0.816	0
	10	80	203.2	0.50	IL2	0.5	−0.289	−0.816	0
Design matrix	11	40	203.2	0.50	IL2	−0.5	−0.289	−0.816	0
	12	60	279.4	0.50	IL2	0	0.577	−0.816	0
	13	60	177.8	1.50	IL2	0	−0.577	0.816	0
	14	40	254.0	1.17	IL3	−0.5	0.289	0.204	0.791
	15	40	203.2	0.83	IL1	−0.5	−0.289	−0.204	−0.791
	16	80	254.0	1.17	IL3	0.5	0.289	0.204	0.791
	17	80	203.2	0.83	IL1	0.5	−0.289	−0.204	−0.791
	18	60	177.8	1.17	IL3	0	−0.577	0.204	0.791
	19	60	279.4	0.83	IL1	0	0.577	−0.204	−0.791
	20	60	228.6	0.67	IL3	0	0	−0.612	0.791
	21	60	228.6	1.33	IL1	0	0	0.612	−0.791

X_1: Temperature; X_2: Pipe diameter; X_3: Fluid velocity; X_4: IL nature. IL1: [omim][Cl]; IL2: [omim][BF4]; IL3: [bmim][SCN]. Dashed lines limit three-factors experimental design for individual fluids (see Computational details)

Table S2. Design matrix ($5^2 = 25$ experiments) for the second computational experiment carried out in the current work. The effect of the temperature and the solvent mole fraction on the transport properties of the mixtures was studied. IL ≡ [omim][Cl]. Solvent ≡ methanol and water. Fluid flow = 10 t/h. Inner pipe diameter = 203.4 mm. Adiabatic transport. Coded variables: X_1 ≡ Temperature, X_2 ≡ Solvent mole fraction in the binary mixture (Solvent + IL).

Experiment	Coded Factors		Physical Variables	
	X_1	X_2	Temp., °C	$x_{Solv.}$, mole
1	0	−0.5	55	0.1
2	−0.5	0	40	0.2
3	0	−1	55	0
4	1	−1	85	0
5	0	0	55	0.2
6	0.5	0	70	0.2
7	−1	0.5	25	0.3
8	−0.5	0.5	40	0.3
9	−0.5	−1	40	0
10	0	0.5	55	0.3
11	0.5	−0.5	70	0.1
12	−0.5	1	40	0.4
13	1	1	85	0.4
14	0.5	−1	70	0
15	−1	0	25	0.2
16	1	−0.5	85	0.1
17	−1	−1	25	0
18	−1	1	25	0.4
19	1	0	85	0.2
20	−1	−0.5	25	0.1
21	0.5	0.5	70	0.3
22	−0.5	−0.5	40	0.1
23	1	0.5	85	0.3
24	0	1	55	0.4
25	0.5	1	70	0.4

Table S3. Assay laboratory data used to create the petroleum fraction used to model the lubricant oil is considered a conventional fluid in this work.

Bulk property		Experimental value	
Density at 15°C, kg/m^3		890	
Kinematic viscosity, cSt		130 (20 °C) 90 (40 °C)	
ASTM D1160 Atmospheric distillation curve			
% Distillate (Volume)	T, °C	% Distillate (Volume)	T, °C
1.0	99.7	60.0	259.9
2.0	127.8	65.0	269.4
3.0	150.7	60.0	259.9
4.0	168.2	65.0	269.4
5.0	177.8	70.0	280.1
7.0	195.5	72.0	284.9
9.0	202.4	73.0	287.5
10.0	206.6	74.0	291.6
15.0	216.4	75.0	294.6
20.0	223.2	76.0	297.2
25.0	227.7	77.0	299.4
30.0	231.3	78.0	303.1

35.0	235.3	79.0	306.2
40.0	238.8	80.0	310.8
45.0	243.1	81.0	315.6
50.0	247.6	82.0	321.2
55.0	254.1	83.0	328.0

In this case, the thermodynamic properties were calculated using the Peng-Robinson equation of state.

Table S4. Methodologies used in this work for the equipment´s sizing and determining the thickness of the thermal insulation used for reducing heat loss through the pipe wall in the fluid transport operations.

Equipment	Sizing method
Heat transfer area (A) of the exchanger	Heat transfer area was determined by the equation: $A = \frac{(U \cdot A)^{Calculated}}{U_{Design}}$ $(U \cdot A)$ was calculated with Aspen HYSYS by the heat exchanger model for the heating conditions. Exchanger model = Simple Weighted (interval analysis for LMTD calculation was used) U_{Design} is a heat transfer coefficient value, typical for the heating service evaluated. A fixed value of 100 W/m^2.K [24] was taken for all the situations calculated
Insulation thickness ($t_{Insulation}$)	Insulation thickness ($t_{Insul.}$) was obtained as the mean value of two different calculations: i)- the required to reduce the heat losses through the pipe wall in 90% respect to the bare pipe. This condition was set by an *Adjust* operator included in the process model ii)- that one obtained by the equation recommended by [24]: $t_{Insul.} = 0.085 \cdot D_{Nom.}^{0.20} \cdot \Delta T^{0.65}$ where: the optimal thickness is given in cm; $D_{Nom.}$ is the bare pipe nominal diameter (in cm), and ΔT is the difference between the temperature of the transported fluid and the ambient (25 °C) To correlate the nominal and the inside diameters. Schedule 40 was selected for the pipe Poly-styrene foam was selected as insulation material due to the low temperatures evaluated The pipe was considered exposed to the air, which velocity was 1 m/s

Table S5. Procedures used to estimate the equipment costs.

Equipment	Cost estimation method
Pipe	The cost ($) of the pipe was taken as the maximum value of those obtained by the next two procedures: 1. A shortcut ponderal method: $Cost = \frac{\pi}{4} \cdot f \cdot L \cdot (D_{Out}^2 - D_{Inn}^2) \cdot \rho \cdot Price$ 2. The equation proposed by [24]: $Cost = L \cdot (0.1922 \cdot D_{Out}^2 + 3.907 \cdot D_{Out} + 22.33)$ where: f = 1.3 is a machinery factor. L and D are the pipe length and the inside diameter. respectively. *Out* and *Ins* design the outer and inner diameters, respectively. ρ and *Price* are the steel density and price, respectively Prices of the carbon steel and the stainless steel S316 were 3.06 and 16.35 $/kg, respectively. They were taken from the Aspen Economics Evaluation database for 2022
Insulation	The insulation cost ($) was obtained as the average for the next two values: 1. The equation given by [24]: $Cost = 1.13 \cdot t_{Insul.} \cdot (D_{Out} + t_{Insul.}) \cdot A \cdot L$ where: $t_{Insul.}$ is the insultation thickness (cm). D_{Out} is the outer diameter of the bare tube (cm). A is the insulation surface (cm^2). L is the pipe length 2. The empirical correlation:

	$Cost = Price \cdot A_{Insul.}$ where: $A_{Insul.}$ is the insulation surface. Price = 25 \$/m^2 is the purchasing price of the insulation (https://www.rockwool.com)
Heat exchanger	$Cost = 7296 \cdot A^{0.65}$ where: the cost is given in \$. A is the heat transfer area (Table 4SM) Equation was adapted from [38]
Pump	$Cost = 1550 \cdot exp(9.2951 - 0.601 \cdot S + 0.0519 \cdot S^2)$ where: the cost is given in \$. and: $S = ln(7.97496 \cdot Qv \cdot h^{0.5})$ where: Qv is the volumetric flow (m^3/h). h is the pump pressure head (m) Equation was adapted from [39]

Table S6. Procedure and prices used to calculate the operating costs.

Service	Price or cost estimation methodology
Low pressure steam for heating the ILs and their mixtures with conventional solvents. T = 125 ºC	The cost of the vapor was taken as the maximum value of those calculated with the following prices: 1. 5.5 \$/t 2. 2.2 x 10^{-6} \$/kJ (taken from the Process Utility Manager in Aspen HYSYS) A scenario with zero heating cost was also considered to account for cases in which the thermal conditioning of the IL is achieved through energy integration using hot process streams
Electricity for pump motor	2.78 x 10^{-5} \$/kJ (0.1 \$/kW.h)
Solvent used as viscosity-reducers	0, 5, 20, 50, and 100 \$/t. See section "Equipment sizing and economic evaluation"

Table S7a. Results from the first experiment conducted in this study (see Computational Details) for some selected ILs. Experiment numbers and conditions correspond to Table 1SM. [bmim][Ac] was also included in the three-factor design for comparison purposes, but not in the 4-factor design.

Experiments 1–13 of the three-factors Doehlert design												
Exper.	[omim][Cl]			[bmim][Ac]			[omim][BF_4]			[bmim][SCN]		
	ΔP, kPa/m	Re	$m_{Solv.}$, t/h	ΔP, kPa/m	Re	$m_{Solv.}$, t/h	ΔP, kPa/m	Re	$m_{Solv.}$, t/h	ΔP, kPa/m	Re	$m_{Solv.}$, t/h
1	0.409	337	146	0.092	3850	151	0.094	4125	156	0.064	14329	151
2	0.079	5286	142	0.055	22477	146	0.063	15995	152	0.049	42130	147
3	14.111	10	150	0.364	404	155	0.208	729	160	0.097	3600	156
4	0.053	1926	255	0.048	13051	264	0.052	11263	275	0.038	33807	265
5	1.208	87	263	0.061	1788	272	0.060	2446	282	0.053	10018	273
6	0.212	963	64	0.117	6525	66	0.127	5632	69	0.092	16904	66
7	4.830	43	66	0.243	894	68	0.184	1223	70	0.130	5009	68
8	0.142	2408	266	0.123	16313	275	0.133	14079	286	0.100	42259	276
9	2.608	109	274	0.138	2235	283	0.205	3058	293	0.136	12522	284
10	0.060	642	57	0.025	4350	59	0.027	3754	61	0.019	11269	59
11	1.358	29	58	0.068	596	60	0.052	815	63	0.027	3337	61
12	0.137	206	109	0.014	2353	113	0.017	2521	117	0.015	8757	113
13	1.015	393	132	0.225	4491	137	0.259	4797	141	0.179	16717	137

Experiments 14 - 21 of the four-factors Doehlert design								
Experiment	14	15	16	17	18	19	20	21
ΔP, kPa/m	0.087	2.870	0.062	0.108	0.113	0.266	0.031	0.637
Re	10676	38	37826	986	14611	292	10806	383
$m_{Solv.}$, t/h	222	97	216	95	107	181	102	194

Table S7b. Results from the first experiment conducted in this study (see Computational Details), involving two conventional solvents selected for comparison with the ILs. Experiment numbers and conditions correspond to those listed in Table 1SM. Only the three-factor design was considered.

Exper.	Diethylene glycol			Water		
	ΔP, kPa/m	Re	$m_{Solv.}$, t/h	ΔP, kPa/m	Re	$m_{Solv.}$, t/h
1	0.056	3302	32	0.033	462557	142
2	0.045	18112	83	0.030	751061	136
3	0.085	221	7	0.037	223533	148
4	0.035	11295	73	0.022	805454	247
5	0.046	1340	22	0.024	444801	257
6	0.081	5647	37	0.051	402727	62
7	0.111	672	11	0.057	222401	64
8	0.090	14119	91	0.060	1006818	257
9	0.119	1679	27	0.066	556002	268
10	0.016	3765	24	0.010	268485	55
11	0.023	448	7	0.011	146961	57
12	0.013	2018	20	0.007	282673	106
13	0.158	3852	38	0.097	539649	129

Table S8. Results of the second computational experiment conducted in this study. The effects of temperature and solvent mole fraction on the transport properties of the mixtures were investigated. IL ≡ [omim][Cl]. Solvent ≡ methanol and water. Details of the experimental conditions are provided in Table 2SM.

Exper.	T, ºC	$x_{Solv.}$, w/w	(Methanol + [omim][Cl])				(Water + [omim][Cl])			
			ΔP, kPa/m	v, m/s	Power, W	Re	ΔP, kPa/m	v, m/s	Power, W	Re
1	55	0.1	0.563	1.042	25.4	250	0.510	1.058	23.3	279
2	40	0.2	0.889	1.222	47.0	185	1.176	1.258	63.9	144
3	55	0	0.791	0.861	29.5	147	0.791	0.861	29.5	147
4	85	0	0.079	0.880	3.0	1493	0.079	0.880	3.0	1493
5	55	0.2	0.337	1.234	18.0	494	0.412	1.270	22.6	415
6	70	0.2	0.139	1.246	7.5	1207	0.159	1.282	8.8	1087
7	25	0.3	1.059	1.408	64.5	179	2.678	1.468	170.0	74
8	40	0.3	0.420	1.421	25.8	456	0.906	1.481	58.0	220
9	40	0	2.947	0.852	108.6	39	2.947	0.852	108.6	39
10	55	0.3	0.182	1.434	11.3	1063	0.340	1.495	22.0	593
11	70	0.1	0.202	1.053	9.2	703	0.180	1.068	8.3	801
12	40	0.4	0.190	1.622	13.4	1149	0.615	1.714	45.6	376
13	85	0.4	0.116	1.667	8.3	8389	0.145	1.761	11.0	4632
14	70	0	0.238	0.870	9.0	493	0.238	0.870	9.0	493
15	25	0.2	2.591	1.211	135.7	63	3.738	1.246	201.4	45
16	85	0.1	0.079	1.064	3.6	1813	0.070	1.079	3.3	2098
17	25	0	12.553	0.844	457.9	9	12.553	0.844	457.9	9
18	25	0.4	0.420	1.607	29.2	516	1.683	1.700	123.7	136
19	85	0.2	0.107	1.259	5.8	2735	0.104	1.294	5.8	2619
20	25	0.1	5.987	1.022	264.5	23	5.665	1.037	254.0	25
21	70	0.3	0.094	1.447	5.9	2300	0.140	1.509	9.1	1456
22	40	0.1	1.734	1.032	77.4	80	1.603	1.047	72.6	88
23	85	0.3	0.120	1.461	7.6	4662	0.138	1.523	9.1	3306
24	55	0.4	0.111	1.637	7.8	2371	0.248	1.729	18.5	942
25	70	0.4	0.136	1.652	9.7	4585	0.111	1.745	8.4	2168

Table S9. Importance of the factors considered in the three-factor design (Table 1SM) in determining the Reynolds number for several ILs and conventional solvents.

Fluid	Factors	
	Temperature	Inside pipe diameter
[bmim][Cl]	68.0	14.2
[omim][Cl]	67.6	14.3
[omim][PF_6]	64.7	15.3
[bmim][Ac]	64.5	15.3
Glycerol	62.6	16.1
[bmpyr][$MetSO_4$]	62.4	16.1
[omim][BF_4]	61.2	16.6
[bupy][BF_4]	61.2	16.6
[hmim][BF_4]	58.3	17.6
[bmim][PF_6]	57.3	18.0
[bmim][BF_4]	56.4	18.4
[emim][$EtSO_4$]	56.1	18.5
[bmim][SCN]	52.6	19.7
Diethylene glycol	50.8	20.2
Water	35.4	26.3

The relative importance of each factor (*Imp.*) is expressed as a percentage. Thus, the importance of the fluid velocity is calculated by: $Imp._{Velocity} = 100 - Imp._{Temperature} - Imp._{Inside\ diameter}$

Nomenclature:
[emim]: 1-ethyl-3-methylimidazolium.
[bmim]: 1-butyl-3-methylimidazolium.
[hmim]: 1-hexyl-3-methylimidazolium.
[omim]: 1-octyl-3-methylimidazolium.
[Cl]: chloride.
[PF_6]: hexafluorophosphate.
[Ac]: acetate.
[$MetSO_4$]: methyl sulfate.
[BF_4]: tetrafluoroborate.
[$EtSO_4$]: ethyl sulfate.
[SCN]: thiocyanate.

Table S10. Results of the optimization exercises conducted under the conditions outlined in Table 3. In all cases studied, the calculated pressure drop was 0.9 kPa/m. The convergence scheme used in Aspen HYSYS was SQP, and comparable results were obtained using the alternative algorithms BOX and Mixed.

Solvent price-Steel type-Heating cost [(1)]	Temperature, ºC	MetOH mass flow, kg/h	Pipe inside diameter, mm	Liquid velocity, m/s	Minimum value of the OF [(2)], k$/a
0$-CS	26.0	844	93.4	0.761	4.229
0$-CS-0$	26.0	844	93.4	0.761	3.330 (23%)
0$-SS	26.0	844	93.4	0.761	5.120
0$-SS-0$	26.0	844	93.4	0.761	4.597 (10%)
5$-CS	26.0	0.1	215.3	0.075	11.319
5$-CS-0$	47.9	0.1	128.8	0.214	9.250 (18%)
5$-SS	26.0	0.1	215.3	0.075	17.012
5$-SS-0$	48.0	0.1	128.6	0.214	11.160 (34%)
20$-CS	26.0	0.1	215.3	0.075	11.203
20$-CS-0$	48.0	0.1	128.1	0.216	9.174 (18%)
20$-SS	26.0	0.1	215.3	0.075	19.889
50$-CS	26.0	0.1	215.3	0.075	11.227
50$-CS-0$	47.9	0.1	128.4	0.215	9.192 (18%)
50$-SS	26.0	0.1	215.3	0.075	17.042
100$-CS	26.0	0.1	215.3	0.075	11.281
100$-SS	26.0	0.1	215.3	0.075	17.072

[(1)]. A heating cost of zero indicates that the thermal conditioning of the IL is achieved through heat integration using hot process streams, without the use of external heating fluids. [(2)]. The values in parentheses indicate the cost savings achieved through heat integration for thermal conditioning of the mixture, compared to similar economic scenarios where steam is used as the heating medium.