Supplementary File

Biogas upgrading through blends of deep eutectic solvent and monoethanol amine: 4 E's analysis (Energy, Exergy, Environmental, and Economic)

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1 Implementation of the physicochemical properties and Vapor-liquid Equilibrium data for ChCl/Urea in Aspen Plus

The correlations and pure component parameters are needed to simulate CO_2 absorption by Deep eutectic solvent ChCl/Urea using the Peng Robinson (PR) model to be incorporated on the Aspen Plus software. The different options are briefly presented and discussed in the following sections.

1.1 Scalar/Critical properties

The critical properties pressure (P_c), temperature (T_c), volume (V_B), molar volume (V_c), and compressibility (Z_c), acentric factor (□), and Molecular weights (M_w) are estimated using the group contribution method proposed by Valderrama *et al.* [1] An estimation of the liquid molar volume at the normal boiling point (v_b) has been made by correlating the critical volume and normal boiling point temperature using the cubic polynomial. Their values, together with the Aspen Plus parameter code, are given in Table S-1

Table S-1 Critical properties of ChCl/Urea

Parameters	**ChCl/Urea**
Molecular Weight (M_w)	86.58
Normal Boiling temperature (T_B)	445.6 K
Critical Temperature (T_C)	644.4 K
Critical Pressure (P_C)	49.35 bar
Critical Volume (V_C)	0.25 m^3/kmol
Acentric factor (□)	0.661
Compressibility factor (Z_c)	0.23
Molar Volume (V_B)	86.87 cc/mol

1.2 Temperature-Dependent Properties

To model components that are not available on the Aspen data bank, we need to specify the temperature-dependent properties of the concerned component in our case, ChCl/Urea. The temperature-dependent properties that need to be specified includes density, viscosity, surface tension, and heat capacity. These properties are evaluated based on the experimental data collected at various temperatures.

1.3 Liquid Molar volume

The experimental density data [2–6] of ChCl/Urea as a function of temperature was used for liquid molar volume calculation by correlating density with molar weight (v_m =ρ/mol.wt). Further on,

the obtained liquid molar volume data is implemented using the IK-CAPE equation (eq.1) on aspen plus to obtain the fitting parameters and coefficients. The liquid molar volume is implemented in Aspen Plus using the VLPO parameter, and coefficients are shown in Table S-2

$$V^{*}{}_{i}^{,l} = C_{1i} + C_{2i}T + C_{3i}T^{2} \qquad \text{eq.1}$$

Table S-2 Fitting parameters for the liquid molar volume VLPO as a function of temperature

VLPO	C_1 / $cm^3 \cdot mol^{-1}$	C_2/ $cm^3 \cdot mol^{-1} \cdot K^{-1}$	C_3 / $cm^3 \cdot mol^{-1} \cdot K^{-2}$
ChCl/Urea	0.0942	2.4×10^{-6}	3.20×10^{-7}

Table S-3 presents the experimental and estimated liquid molar volume and deviation between the experimental and estimated data.

Table S-3 Experimental and predicted molar volume (Vm) of ChCl/Urea as a function of temperature

$V_{m(exp)}$	$V_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
72.439	72.17433	0.72439	-0.26467	30	30.00012	0.1	0.000123
72.59769	72.30467	0.725977	-0.29302	35	35.00015	0.1	0.000154
72.7563	72.45105	0.727563	-0.30526	40	40.00018	0.1	0.000178
72.91561	72.61347	0.729156	-0.30215	45	45.00019	0.1	0.000194
73.07562	72.79193	0.730756	-0.28369	50	50.0002	0.1	0.000198
73.23634	72.98643	0.732363	-0.2499	55	55.00019	0.1	0.000189
73.39776	73.19698	0.733978	-0.20078	60	60.00016	0.1	0.000163
73.5599	73.42357	0.735599	-0.13633	65	65.00012	0.1	0.000118
73.72275	73.66619	0.737228	-0.05656	70	70.00005	0.1	5.22E-05
73.88633	73.92486	0.738863	0.038529	75	74.99996	0.1	-3.77E-05
74.0633	74.19957	0.740633	0.136263	80	79.99986	0.1	-0.00014
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
71.05458	72.06002	0.710546	1.005449	25	24.99958	0.1	-0.00042
71.70186	72.61344	0.717019	0.911577	45	44.9994	0.1	-0.0006
72.48221	73.19695	0.724822	0.714736	60	59.99941	0.1	-0.00059
73.55365	74.19954	0.735536	0.645886	80	79.99932	0.1	-0.00068
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
72.27648	72.06004	0.722765	-0.21645	25	25.00009	0.1	8.81E-05
72.43976	72.17433	0.724398	-0.26543	30	30.00012	0.1	0.000124
72.5916	72.30467	0.725916	-0.28693	35	35.00015	0.1	0.000151
72.75019	72.45105	0.727502	-0.29914	40	40.00017	0.1	0.000175
72.90947	72.61347	0.729095	-0.29601	45	45.00019	0.1	0.00019
73.06946	72.79193	0.730695	-0.27753	50	50.00019	0.1	0.000194
73.23014	72.98643	0.732301	-0.24371	55	55.00018	0.1	0.000184
73.39154	73.19698	0.733915	-0.19456	60	60.00016	0.1	0.000158
$v_{m(exp)}$	$v_{m(est)}$	Standard	deviation	T_{exp}	T_{est}	Standard deviation	Difference

		deviation					
72.14399	71.96178	0.72144	-0.18221	20	20.00006	0.1	6.32E-05
72.48221	72.17433	0.724822	-0.30788	30	30.00014	0.1	0.000143
72.83587	72.45105	0.728359	-0.38482	40	40.00022	0.1	0.000224
73.18063	72.79193	0.731806	-0.38869	50	50.00027	0.1	0.000271
73.54115	73.19698	0.735412	-0.34417	60	60.00028	0.1	0.000278
73.94944	73.6662	0.739494	-0.28323	70	70.00026	0.1	0.00026
74.41341	74.19959	0.744134	-0.21382	80	80.00022	0.1	0.000218
74.93509	74.79714	0.749351	-0.13795	90	90.00015	0.1	0.000155
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
72.56726	72.06004	0.725673	-0.50722	25	25.0002	0.1	0.000205
72.48828	72.06004	0.724883	-0.42824	25	25.00017	0.1	0.000173
72.40947	72.06004	0.724095	-0.34943	25	25.00014	0.1	0.000142
72.33083	72.06004	0.723308	-0.27079	25	25.00011	0.1	0.00011
72.24633	72.06004	0.722463	-0.18629	25	25.00008	0.1	7.59E-05
72.16804	72.06003	0.72168	-0.10801	25	25.00004	0.1	4.41E-05
72.08993	72.06003	0.720899	-0.02989	25	25.00001	0.1	1.22E-05
72.01797	72.06003	0.72018	0.042066	25	24.99998	0.1	-1.72E-05
71.94615	72.06003	0.719462	0.11388	25	24.99995	0.1	-4.68E-05
71.87448	72.06003	0.718745	0.185551	25	24.99992	0.1	-7.64E-05
71.80295	72.06003	0.71803	0.257079	25	24.99989	0.1	-0.00011
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
72.44582	72.17433	0.724458	-0.27149	30	30.00013	0.1	0.000127
72.3671	72.17433	0.723671	-0.19277	30	30.00009	0.1	9.01E-05
72.27648	72.17433	0.722765	-0.10216	30	30.00005	0.1	4.79E-05
72.20415	72.17433	0.722042	-0.02983	30	30.00001	0.1	1.40E-05
72.12596	72.17433	0.72126	0.048369	30	29.99998	0.1	-2.28E-05
72.04194	72.17433	0.720419	0.132389	30	29.99994	0.1	-6.24E-05
71.96409	72.17433	0.719641	0.210232	30	29.9999	0.1	-9.93E-05
71.88642	72.17432	0.718864	0.287908	30	29.99986	0.1	-0.00014
71.81486	72.17432	0.718149	0.359459	30	29.99983	0.1	-0.00017
71.74345	72.17432	0.717435	0.430869	30	29.9998	0.1	-0.0002
71.67219	72.17432	0.716722	0.502136	30	29.99976	0.1	-0.00024
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
72.62204	72.30467	0.72622	-0.31738	35	35.00017	0.1	0.000167
72.53686	72.30467	0.725369	-0.2322	35	35.00012	0.1	0.000122
72.45795	72.30467	0.724579	-0.15328	35	35.00008	0.1	8.08E-05
72.37315	72.30466	0.723732	-0.06849	35	35.00004	0.1	3.62E-05
72.29459	72.30466	0.722946	0.010074	35	34.99999	0.1	-5.34E-06
72.2162	72.30466	0.722162	0.088464	35	34.99995	0.1	-4.70E-05
72.13197	72.30466	0.72132	0.172694	35	34.99991	0.1	-9.19E-05
72.05993	72.30466	0.720599	0.244735	35	34.99987	0.1	-0.00013
71.98204	72.30466	0.71982	0.322617	35	34.99983	0.1	-0.00017
71.9103	72.30466	0.719103	0.394359	35	34.99979	0.1	-0.00021
71.84466	72.30466	0.718447	0.459997	35	34.99975	0.1	-0.00025
$v_{m(exp)}$	$v_{m(est)}$	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference

72.79913	72.45105	0.727991	-0.34808	40	40.0002	0.1	0.000203
72.71353	72.45105	0.727135	-0.26248	40	40.00015	0.1	0.000153
72.63423	72.45104	0.726342	-0.18318	40	40.00011	0.1	0.000107
72.54902	72.45104	0.72549	-0.09798	40	40.00006	0.1	5.75E-05
72.47008	72.45104	0.724701	-0.01903	40	40.00001	0.1	1.12E-05
72.38525	72.45104	0.723853	0.065788	40	39.99996	0.1	-3.88E-05
72.30666	72.45104	0.723067	0.144374	40	39.99991	0.1	-8.53E-05
72.22825	72.45104	0.722282	0.22279	40	39.99987	0.1	-0.00013
72.15	72.45104	0.7215	0.301036	40	39.99982	0.1	-0.00018
72.07792	72.45103	0.720779	0.373113	40	39.99978	0.1	-0.00022
72.01198	72.45103	0.72012	0.439056	40	39.99974	0.1	-0.00026

1.4 Viscosity

The viscosity (η) experimental data[2,4–7] as a function of temperature was implemented in aspen plus using Andrade equation eq.2

$$\ln(\eta) = C_{1i} + \frac{C_{2i}}{T} + c_{3i}\ln(T) \qquad eq.2$$

Further on, the obtained viscosity data is implemented using the DIPPR equation (eq.2) on aspen plus to obtain the fitting parameters and coefficients. The viscosity is implemented in Aspen Plus using the MULAND parameter, and fitted coefficients are shown in table S-4.

Table S-4 Fitting parameters for the viscosity (η) MULAND as a function of temperature

	C_1	C_2 / K	C_3
ChCl/Urea	-443.789	1.97×10^4	40.4835

Table S-5 presents the experimental and estimated viscosity and deviation between the experimental and estimated data

Table S-5 Experimental and predicted viscosity (η) of ChCl/Urea as a function of temperature

η_{exp}	η_{est}	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
748.09	777.2035	7.4809	29.11353	25	25.19355	0.1	0.193554
511.61	509.6518	5.1161	-1.95816	30	29.98126	0.1	-0.01874
351.46	342.5035	3.5146	-8.95649	35	34.87765	0.1	-0.12235
243.04	235.572	2.4304	-7.46801	40	39.85544	0.1	-0.14456
119.81	118.8758	1.1981	-0.93417	50	49.96466	0.1	-0.03534
86.092	87.01971	0.86092	0.927706	55	55.04793	0.1	0.047932
63.202	64.89764	0.63202	1.695641	60	60.11676	0.1	0.116761
47.644	49.26169	0.47644	1.617685	65	65.14363	0.1	0.143626
37.039	38.02477	0.37039	0.985769	70	70.10826	0.1	0.108262

29.79	29.82174	0.2979	0.031738	75	75.0041	0.1	0.004105
24.808	23.74449	0.24808	-1.06351	80	79.84647	0.1	-0.15353
169.57	165.6164	1.6957	-3.95364	45	44.89238	0.1	-0.10762
η_{exp}	η_{est}	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
750	787.4109	7.5	37.41087	24.85	25.09836	0.1	0.248362
449	515.9569	4.49	66.95688	29.85	30.59427	0.1	0.744266
330	346.4926	3.3	16.49261	34.85	35.09445	0.1	0.244452
231	238.1545	2.31	7.154466	39.85	39.99861	0.1	0.148612
161	167.3248	1.61	6.324789	44.85	45.03551	0.1	0.185508
119	120.0293	1.19	1.029333	49.85	49.8895	0.1	0.039503
95	87.81366	0.95	-7.18634	54.85	54.52765	0.1	-0.32235
η_{exp}	η_{est}	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
1371.972	1209.339	13.71972	-162.633	20	19.42313	0.1	-0.57688
527.2786	509.6518	5.272786	-17.6268	30	29.83737	0.1	-0.16263
238.0763	235.572	2.380763	-2.50431	40	39.95017	0.1	-0.04983
119.8049	118.8758	1.198049	-0.92907	50	49.96485	0.1	-0.03515
68.6478	64.89764	0.686478	-3.75016	60	59.77231	0.1	-0.22769
41.9612	38.02477	0.419612	-3.93643	70	69.64684	0.1	-0.35316
28.1053	23.74449	0.281053	-4.36081	80	79.49257	0.1	-0.50743
19.949	15.46116	0.19949	-4.48784	90	89.34189	0.1	-0.65811
η_{exp}	η_{est}	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
1571	1209.339	15.71	-361.661	20	18.92316	0.1	-1.07684
953.7	509.6518	9.537	-444.048	30	28.2915	0.1	-1.7085
608.4	342.5035	6.084	-265.896	35	33.40488	0.1	-1.59512
403.2	235.572	4.032	-167.628	40	38.50653	0.1	-1.49347
277.2	165.6164	2.772	-111.584	45	43.59232	0.1	-1.40768
195.9	118.8758	1.959	-77.0242	50	48.6695	0.1	-1.3305
143.6	87.01971	1.436	-56.5803	55	53.72788	0.1	-1.27212
107.7	64.89764	1.077	-42.8024	60	58.78237	0.1	-1.21764

1.5 Molar liquid Heat Capacity

The Aspen Plus property method calculates the molar heat capacity of the liquid state based on the slope of the enthalpy of the liquid state (H^l) as a function of temperature. the molar liquid heat capacity is implemented in Aspen Plus based on DIPPR equation. The fitting parameters and the coefficient for molar liquid heat capacity as mentioned by ma et. al[8] were implemented in Aspen Plus as the CPLDIP parameter are shown in Table S-6

Table S-6 parameters for molar heat capacity CPLDIP[8]

	C_1/ j mol^{-1}	C_2 / j mol^{-1} K^{-1}	C_3/ j mol^{-1}K^{-2}
ChCl/Urea	117.3	0.2085	1.679×10^{-12}

1.6 Surface Tension

The surface tension (σ) data[8] for ChCl/Urea was obtained using Macleod equation (eq.3) as explained by Shahbaz et. al[9]

$$\sigma^{1/4} = \frac{P_{parachor} \times \rho}{Mol.wt} \qquad \text{eq.3}$$

The theoretical surface tensions estimation was also calculated by Ma et. al[8] which was used to determine surface tension parameters on Aspen Plus using DIPPR eq. 4. The fitting parameters and the coefficient for surface tension obtained and implemented in Aspen Plus as the SIGDIP parameter are shown in Table S-7

$$\sigma^{*,l}_i = C_{1i}(1 - T_{ri})^{\left(C_{2i} + C_{3i}T_{ri} + C_{4i}T_{ri}^2 + C_{5i}T_{ri}^3\right)} \qquad \text{eq.4}$$

Table S-7 Fitting parameters for the surface tension (σ) SIGDIP as a function of temperature

	a_3 / N·m^{-1}	b_3 / N·m^{-1}·K^{-1}
ChCl/Urea	0.08248	0.60

Table S-8 presents the experimental and estimated surface tension and deviation of the SIGDIP model from experimental surface tension.

Table S-8 Experimental and predicted surface tension of ChCl/Urea as a function of temperature

σ_{exp}	σ_{est}	Standard deviation	deviation	T_{exp}	T_{est}	Standard deviation	Difference
63.76	63.74696	0.63	-0.013	25	24.99	0.1	-3.62E-05
63.19	63.18247	0.63	-0.007	30	29.99	0.1	-2.13E-05
62.61	62.61798	0.62	0.0079	35	35	0.1	2.30E-05
62.04	62.05348	0.62	0.013	40	40	0.1	3.96E-05
61.48	61.48899	0.61	0.0089	45	45	0.1	2.69E-05
60.92	60.92451	0.60	0.0045	50	50	0.1	1.37E-05
60.36	60.36002	0.60	1.70E-05	55	55	0.1	5.28E-08
59.81	59.79553	0.59	-0.014	60	59.99	0.1	-4.57E-05

2 Vapor-liquid equilibrium

The experimentally determined vapor-liquid equilibrium (VLE) data of the systems CO_2 + ChCl/Urea, CH_4 + ChCl/Urea, and MEA + ChcCl/Urea are implemented in Aspen Plus using the Peng Robinson (PR) thermodynamic model.

The system ChCl/Urea + CH_4 phase behaviour at a temperature range of 35.05-80.05 °C up to pressures of 36.18 bar was determined. The phase behaviour of the system ChCl/Urea + MEA at temperature 40.05-80.05 °C up to the pressure of 8.55 bar. The system ChCl/Urea + CO_2 phase behaviour at temperature 35.05-80.05 °C and pressure up to 36.18 bar. The VLE data were fitted to the PR model using Aspen Plus as shown in following Tables.

Table S-9 The experimental and predicted CH_4 solubility (X_{CH4}) in ChCl/Urea as a function of pressure

$X_{CH4(exp)}$	$X_{CH4(est)}$	Standard deviation	Difference	P_{exp}	P_{est}	Standard deviation	Difference	Ref
35.05 °C								
0.014	0.014	1.4E-05	1.52E-05	5.85	5.8244	0.00585	-0.0255	[10]
0.029	0.0296	2.9E-05	0.00059	12.74	12.4727	0.01274	-0.2673	
0.049	0.0485	4.9E-05	-0.00044	20.42	20.5853	0.02042	0.16528	
0.068	0.066	6.8E-05	-0.00154	27.82	28.4227	0.02782	0.60267	
0.089	0.0856	8.9E-05	-0.0034	35.7	36.9753	0.0357	1.27532	
Average deviation = -0.0009 Root mean square error = 0.0017 Average absolute = 0.0012								
40.05 °C								
7e-05	6.3e-05	7E-08	-7.45E-06	0.134	0.1485	0.00013	0.01454	[11]
0.00028	0.00025	2.8E-07	-2.92E-05	0.527	0.5812	0.00052	0.05424	
0.00057	0.000512	5.7E-07	-5.81E-05	1.076	1.1828	0.00107	0.10687	
0.00081	0.00073	8.1E-07	-8.09E-05	1.536	1.6847	0.00153	0.14871	
0.0011	0.001	1.1E-06	-0.00012	2.028	2.2553	0.00202	0.22737	
Average deviation = -5.9e-05 Root mean square error = 7.2e-05 Average absolute = 5.9e-05								
45.05 °C								
0.013	0.0128	1.3E-05	-0.00021	5.48	5.5535	0.0055	0.07355	[10]
0.028	0.0284	2.8E-05	0.00036	12.68	12.5098	0.01268	-0.17017	
0.044	0.0444	4.4E-05	0.00045	20.01	19.8130	0.02001	-0.19695	
0.063	0.0628	6.3E-05	-0.00021	28.18	28.2773	0.02818	0.09737	
0.081	0.0802	8.1E-05	-0.00083	36.18	36.523	0.03618	0.34321	
Average deviation = -8.8e-05 Root mean square error = 0.00047 Average absolute = 0.00041								
50.05 °C								
5E-05	4.598E-05	5E-08	-4.02E-06	0.101	0.1091	0.0001	0.00818	[11]
0.00024	0.000231	2.4E-07	-8.63E-06	0.511	0.5233	0.0005	0.01235	

0.00049	0.00047	4.9E-07	-2.46E-05	1.005	1.0447	0.0010	0.03968	
0.00071	0.0007	7.1E-07	-2.02E-05	1.526	1.5497	0.0015	0.02370	
0.00095	0.00092	9.5E-07	-3.15E-05	2.021	2.0626	0.0020	0.04162	
Average deviation = -1.8e-05 Root mean square error = 2.05e-05 Average absolute = 1.78e-05								
55.05 °C								
0.012	0.01203	1.2E-05	3.200E-05	5.5	5.475	0.0055	-0.0242	[10]
0.026	0.0268	2.6E-05	0.000757	12.7	12.34	0.0127	-0.3557	
0.041	0.0423	4.1E-05	0.001284	20.31	19.724	0.02031	-0.5859	
0.059	0.0592	5.9E-05	0.000195	27.9	27.830	0.0279	-0.0697	
0.076	0.07575	7.6E-05	-0.00025	35.9	36.021	0.0359	0.12111	
Average deviation = 0.000403 Root mean square error = 0.00068 Average absolute = 0.000503								
60.05 °C								
5E-05	4.7E-05	5E-08	-2.57E-06	0.107	0.1123	0.0001	0.00534	[11]
0.00021	0.000218	2.1E-07	7.86E-06	0.507	0.4821	0.0005	-0.02487	
0.00042	0.00043	4.2E-07	1.84E-05	1.017	0.9607	0.0010	-0.05626	
0.00059	0.0006	5.9E-07	4.11E-05	1.501	1.3827	0.0015	-0.11821	
0.0008	0.00085	8E-07	5.09E-05	2.009	1.8618	0.0020	-0.14717	
Average deviation = 2.3e-05 Root mean square error = 3.1e-05 Average absolute = 2.4e-05								
80.05 °C								
4E-05	4.00E-05	4E-08	1.31E-08	0.106	0.1054	0.0001	-0.00057	[11]
0.00017	0.000198	1.7E-07	2.81E-05	0.505	0.4250	0.0005	-0.07994	
0.00033	0.00039	3.3E-07	6.93E-05	1.029	0.8356	0.0010	-0.19337	
0.00048	0.0005	4.8E-07	0.000105	1.506	1.2158	0.0015	-0.29017	
0.00063	0.0007	6.3E-07	0.000142	1.996	1.6018	0.0019	-0.39413	
Average deviation = 6.89e-05 Root mean square error = 8.58e-05 Average absolute = 6.9e-05								

Table S-10 The experimental and predicted CO_2 solubility (X_{CO2}) in ChCl/Urea as a function of pressure

$X_{CO2(exp)}$	$X_{CO2(est)}$	Standard deviation	Difference	P_{exp}	P_{est}	Standard deviation	Difference	Ref
40.05 °C								
0.038	0.029471	3.80E-05	-0.00853	0.301	0.395293	0.000301	0.094293	[12]
0.04	0.036805	4.00E-05	-0.0032	0.763	0.871693	0.000763	0.108693	
0.048	0.044664	4.80E-05	-0.00334	0.993	1.120986	0.000993	0.127986	
0.056	0.05512	5.60E-05	-0.00088	1.779	1.906954	0.001779	0.127954	
0.065	0.065062	6.50E-05	6.19E-05	2.413	2.541677	0.002413	0.128677	
0.077	0.078258	7.70E-05	0.001258	3.327	3.44676	0.003327	0.11976	
0.087	0.090037	8.70E-05	0.003037	4.634	4.709407	0.004634	0.075407	
0.094	0.097853	9.40E-05	0.003853	5.333	5.38442	0.005333	0.05142	
0.101	0.105989	0.000101	0.004989	6.314	6.319263	0.006314	0.005263	
0.108	0.114201	0.000108	0.006201	7.412	7.35709	0.007412	-0.05491	
0.111	0.117675	0.000111	0.006675	7.841	7.761446	0.007841	-0.07955	
0.035	0.031846	3.50E-05	-0.00315	0.62	0.716294	0.00062	0.096294	

0.038	0.035778	3.80E-05	-0.00222	0.848	0.950404	0.000848	0.102404	
0.048	0.047218	4.80E-05	-0.00078	1.54	1.655133	0.00154	0.115133	
0.057	0.057738	5.70E-05	0.000738	2.551	2.66112	0.002551	0.11012	
0.067	0.068139	6.70E-05	0.001139	3.154	3.271123	0.003154	0.117123	
0.074	0.075815	7.40E-05	0.001815	3.871	3.980982	0.003871	0.109982	
0.081	0.083992	8.10E-05	0.002992	5.177	5.253719	0.005177	0.076719	
0.087	0.090668	8.70E-05	0.003668	6.067	6.120498	0.006067	0.053498	
0.095	0.099178	9.50E-05	0.004178	6.736	6.778688	0.006736	0.042688	
0.1	0.104742	0.0001	0.004742	7.484	7.502678	0.007484	0.018678	
0.103	0.108163	0.000103	0.005163	8.061	8.057551	0.008061	-0.00345	
0.043	0.043002	4.30E-05	2.15E-06	1.28	1.480955	0.00128	0.200955	
0.051	0.052337	5.10E-05	0.001337	2.024	2.299884	0.002024	0.275884	
0.06	0.063019	6.00E-05	0.003019	3.204	3.574266	0.003204	0.370266	
0.069	0.073188	6.90E-05	0.004188	4.045	4.481802	0.004045	0.436802	
0.074	0.07892	7.40E-05	0.00492	4.579	5.052136	0.004579	0.473136	
0.082	0.088136	8.20E-05	0.006136	5.454	5.980112	0.005454	0.526112	
0.088	0.095419	8.80E-05	0.007419	6.603	7.170314	0.006603	0.567314	
0.097	0.106157	9.70E-05	0.009157	8.096	8.701864	0.008096	0.605864	
Average deviation = 0.002513 Root mean square error =0.004348 Average absolute = 0.003626								
60.05 °C								
0.034	0.028574	3.40E-05	-0.00543	0.54	0.679387	0.00054	0.139387	12
0.036	0.030796	3.60E-05	-0.0052	0.626	0.775882	0.000626	0.149882	
0.039	0.03395	3.90E-05	-0.00505	0.746	0.910628	0.000746	0.164628	
0.05	0.04689	5.00E-05	-0.00311	1.608	1.834438	0.001608	0.226438	
0.058	0.056516	5.80E-05	-0.00148	2.619	2.877058	0.002619	0.258058	
0.066	0.065322	6.60E-05	-0.00068	3.509	3.788163	0.003509	0.279163	
0.074	0.073993	7.40E-05	-7.18E-06	4.41	4.70283	0.00441	0.29283	
0.085	0.085675	8.50E-05	0.000675	5.532	5.837498	0.005532	0.305498	
0.094	0.095168	9.40E-05	0.001168	6.4	6.711695	0.0064	0.311695	
0.1	0.101887	0.0001	0.001887	7.33	7.628413	0.00733	0.298413	
0.104	0.106359	0.000104	0.002359	7.96	8.246404	0.00796	0.286404	
0.107	0.109831	0.000107	0.002831	8.567	8.836355	0.008567	0.269355	
0.032	0.02941	3.20E-05	-0.00259	0.866	1.012059	0.000866	0.146059	
0.035	0.032007	3.50E-05	-0.00299	0.918	1.076268	0.000918	0.158268	
0.042	0.040009	4.20E-05	-0.00199	1.525	1.719997	0.001525	0.194997	
0.048	0.045742	4.80E-05	-0.00226	1.759	1.979229	0.001759	0.220229	
0.055	0.053799	5.50E-05	-0.0012	2.601	2.849773	0.002601	0.248773	
0.061	0.060587	6.10E-05	-0.00041	3.451	3.718228	0.003451	0.267228	
0.068	0.06817	6.80E-05	0.00017	4.355	4.639489	0.004355	0.284489	
0.08	0.080786	8.00E-05	0.000786	5.692	6.001341	0.005692	0.309341	
0.084	0.085453	8.40E-05	0.001453	6.7	7.002405	0.0067	0.302405	
0.091	0.092609	9.10E-05	0.001609	7.282	7.597776	0.007282	0.315776	
0.098	0.100062	9.80E-05	0.002062	8.245	8.561303	0.008245	0.316303	
0.102	0.104488	0.000102	0.002488	9.036	9.342752	0.009036	0.306752	
0.036	0.034662	3.60E-05	-0.00134	0.951	1.157926	0.000951	0.206926	
0.043	0.043498	4.30E-05	0.000498	1.88	2.21285	0.00188	0.33285	
0.047	0.047902	4.70E-05	0.000902	2.2	2.579592	0.0022	0.379592	
0.053	0.054921	5.30E-05	0.001921	2.988	3.464567	0.002988	0.476567	
0.061	0.063981	6.10E-05	0.002981	3.846	4.428077	0.003846	0.582077	
0.07	0.074666	7.00E-05	0.004666	5.35	6.079755	0.00535	0.729755	
0.081	0.087478	8.10E-05	0.006478	6.856	7.723377	0.006856	0.867377	

0.091	0.099146	9.10E-05	0.008146	8.086	9.057687	0.008086	0.971687	
0.097	0.106454	9.70E-05	0.009454	9.246	10.2853	0.009246	1.039304	
Average deviation = 0.000569 Root mean square error =0.003439 Average absolute = 0.002614								
80.05 °C								
0.029	0.021359	2.90E-05	-0.00764	0.344	0.491711	0.000344	0.147711	12
0.03	0.024094	3.00E-05	-0.00591	0.485	0.648813	0.000485	0.163813	
0.046	0.041524	4.60E-05	-0.00448	1.572	1.89787	0.001572	0.32587	
0.054	0.050585	5.40E-05	-0.00342	2.513	2.925459	0.002513	0.412459	
0.062	0.058952	6.20E-05	-0.00305	3.33	3.810998	0.00333	0.480998	
0.07	0.06784	7.00E-05	-0.00216	4.57	5.118365	0.00457	0.548365	
0.081	0.078661	8.10E-05	-0.00234	5.43	6.047786	0.00543	0.617786	
0.09	0.088202	9.00E-05	-0.0018	6.668	7.337794	0.006668	0.669794	
0.097	0.095792	9.70E-05	-0.00121	7.83	8.530879	0.00783	0.700879	
0.031	0.02611	3.10E-05	-0.00489	0.662	0.852072	0.000662	0.190072	
0.033	0.02859	3.30E-05	-0.00441	0.85	1.067847	0.00085	0.217847	
0.042	0.038824	4.20E-05	-0.00318	1.715	2.030263	0.001715	0.315263	
0.046	0.04309	4.60E-05	-0.00291	2.111	2.464947	0.002111	0.353947	
0.051	0.048582	5.10E-05	-0.00242	2.747	3.151061	0.002747	0.404061	
0.06	0.057542	6.00E-05	-0.00246	3.493	3.967209	0.003493	0.474209	
0.067	0.065309	6.70E-05	-0.00169	4.68	5.216322	0.00468	0.536322	
0.075	0.073875	7.50E-05	-0.00112	5.984	6.579331	0.005984	0.595331	
0.084	0.083215	8.40E-05	-0.00078	7.266	7.917324	0.007266	0.651324	
0.091	0.090499	9.10E-05	-0.0005	8.328	9.017448	0.008328	0.689448	
0.096	0.095486	9.60E-05	-0.00051	8.834	9.550328	0.008834	0.716328	
0.04	0.03969	4.00E-05	-0.00031	1.765	2.167199	0.001765	0.402199	
0.044	0.044528	4.40E-05	0.000528	2.373	2.877248	0.002373	0.504248	
0.05	0.051022	5.00E-05	0.001022	2.836	3.430036	0.002836	0.594036	
0.054	0.055565	5.40E-05	0.001565	3.285	3.956198	0.003285	0.671198	
0.063	0.06624	6.30E-05	0.00324	4.714	5.600502	0.004714	0.886502	
0.07	0.074719	7.00E-05	0.004719	6.083	7.149785	0.006083	1.066785	
0.079	0.085322	7.90E-05	0.006322	7.412	8.653094	0.007412	1.241094	
0.088	0.096054	8.80E-05	0.008054	8.757	10.16019	0.008757	1.40319	
Average deviation = -0.00113 Root mean square error =0.003633 Average absolute = 0.002951								
35.05 °C								
0.05	0.048647	5.00E-05	-0.00135	6.51	6.641574	0.00651	0.131574	13
0.095	0.098734	9.50E-05	0.003734	15.27	14.67166	0.01527	-0.59834	
0.137	0.14732	0.000137	0.01032	24.53	22.84695	0.02453	-1.68305	
0.174	0.192875	0.000174	0.018875	34.45	31.14858	0.03445	-3.30142	
0.195	0.224168	0.000195	0.029168	43.76	38.09109	0.04376	-5.66891	
Average deviation = 0.0121 Root mean square error = 0.016 Average absolute = 0.0126								
45.05 °C								
0.044	0.044031	4.40E-05	3.12E-05	7.06	7.019078	0.00706	-0.04092	13
0.092	0.095709	9.20E-05	0.003709	16.61	15.9564	0.01661	-0.6536	
0.127	0.137888	0.000127	0.010888	26.18	24.17246	0.02618	-2.00754	
0.168	0.183311	0.000168	0.015311	35.27	32.42382	0.03527	-2.84618	
0.188	0.213575	0.000188	0.025575	45.04	39.749	0.04504	-5.291	
Average deviation = 0.01110								

Root mean square error = 0.0142 Average absolute = 0.01110								
55.05 °C								
0.042	0.040917	4.20E-05	-0.00108	6.92	7.06432	0.00692	0.14432	13
0.088	0.090244	8.80E-05	0.002244	16.91	16.47835	0.01691	-0.43165	
0.118	0.125716	0.000118	0.007716	25.44	23.93303	0.02544	-1.50697	
0.156	0.169415	0.000156	0.013415	35.77	33.05895	0.03577	-2.71105	
0.175	0.197131	0.000175	0.022131	44.99	40.10015	0.04499	-4.88985	
Average deviation = 0.0088 Root mean square error = 0.012 Average absolute = 0.0093								
40.05 °C								
0.001	0.000921	1.00E-06	-7.88E-05	0.116	0.124534	0.000116	0.008534	11
0.00417	0.003954	4.17E-06	-0.00022	0.534	0.55738	0.000534	0.02338	
0.00843	0.007883	8.43E-06	-0.00055	1.03	1.089421	0.00103	0.059421	
0.01257	0.011785	1.26E-05	-0.00079	1.548	1.633592	0.001548	0.085592	
0.01624	0.015278	1.62E-05	-0.00096	2.022	2.127143	0.002022	0.105143	
Average deviation = -0.00052 Root mean square error =0.000616 Average absolute = 0.000518								
50.05 °C								
0.00091	0.000844	9.10E-07	-6.63E-05	0.122	0.130482	0.000122	0.008482	11
0.00338	0.003278	3.38E-06	-0.0001	0.523	0.535032	0.000523	0.012032	
0.00655	0.006407	6.55E-06	-0.00014	1.039	1.054093	0.001039	0.015093	
0.00967	0.00946	9.67E-06	-0.00021	1.533	1.555299	0.001533	0.022299	
0.01244	0.012262	1.24E-05	-0.00018	2.017	2.032	0.002017	0.015	
Average deviation = -0.00014 Root mean square error =0.000149 Average absolute = 0.00014								
60.05 °C								
0.00058	0.000565	5.80E-07	-1.50E-05	0.105	0.107291	0.000105	0.002291	11
0.00272	0.002713	2.72E-06	-7.02E-06	0.512	0.510335	0.000512	-0.00167	
0.00557	0.00555	5.57E-06	-1.99E-05	1.038	1.035685	0.001038	-0.00232	
0.00827	0.008299	8.27E-06	2.86E-05	1.57	1.556037	0.00157	-0.01396	
0.0107	0.010698	1.07E-05	-1.56E-06	2.008	1.997361	0.002008	-0.01064	
Average deviation = -2.98e-6 Root mean square error =1.73e-5 Average absolute = 1.44e-5								
80.05 °C								
0.00038	0.000382	3.80E-07	1.59E-06	0.11	0.109136	0.00011	-0.00086	11
0.00199	0.002063	1.99E-06	7.29E-05	0.523	0.50218	0.000523	-0.02082	
0.004	0.004124	4.00E-06	0.000124	1.001	0.967301	0.001001	-0.0337	
0.00621	0.006435	6.21E-06	0.000225	1.558	1.498768	0.001558	-0.05923	
0.00795	0.008276	7.95E-06	0.000326	2.011	1.926148	0.002011	-0.08485	
Average deviation = 0.0015 Root mean square error =0.000188 Average absolute = 0.0015								

Table S-11 The experimental and predicted H_2S solubility (X_{H2S}) in ChCl/Urea as a function of pressure

$X_{H2S(exp)}$	$X_{H2S(est)}$	Standard deviation	Difference	P_{exp}	P_{est}	Standard deviation	Difference	Ref
40.05 °C								
0.00258	0.002593	2.58E-06	1.32E-05	0.117	0.115602	0.000117	-0.0014	11

0.01244	0.012372	1.24E-05	-6.75E-05	0.524	0.522848	0.000524	-0.00115	
0.02352	0.023424	2.35E-05	-9.64E-05	0.994	0.990715	0.000994	-0.00329	
0.03587	0.03579	3.59E-05	-7.96E-05	1.526	1.518574	0.001526	-0.00743	
0.0464	0.046452	4.64E-05	5.18E-05	2.004	1.98837	0.002004	-0.01563	
Average deviation = -0.000035 Root mean square error = 0.000067 Average absolute = 0.000061								
50.05 °C								
0.0096	0.009622	9.60E-06	2.15E-05	0.511	0.506552	0.000511	-0.00445	11
0.01992	0.019778	1.99E-05	-0.00014	1.005	1.005255	0.001005	0.000255	
0.0293	0.029293	2.93E-05	-6.87E-06	1.526	1.516698	0.001526	-0.0093	
0.03834	0.038444	3.83E-05	0.000104	2.021	2.003442	0.002021	-0.01756	
Average deviation = -0.0000058 Root mean square error = 0.000088 Average absolute = 0.000068								
60.05°C								
0.00777	0.007854	7.77E-06	8.41E-05	0.517	0.508638	0.000517	-0.00836	11
0.01567	0.01574	1.57E-05	6.99E-05	1.002	0.991925	0.001002	-0.01008	
0.02395	0.024111	2.40E-05	0.000161	1.541	1.522439	0.001541	-0.01856	
0.02993	0.030413	2.99E-05	0.000483	2.005	1.963605	0.002005	-0.0414	
Average deviation = 0.000199 Root mean square error = 0.00026 Average absolute = 0.00019								
80.05°C								
0.00151	0.001451	1.51E-06	-5.87E-05	0.116	0.120695	0.000116	0.004695	11
0.00591	0.005903	5.91E-06	-7.09E-06	0.523	0.521307	0.000523	-0.00169	
0.01182	0.011745	1.18E-05	-7.51E-05	1.001	1.002747	0.001001	0.001747	
0.0168	0.016935	1.68E-05	0.000135	1.501	1.482713	0.001501	-0.01829	
0.02269	0.022871	2.27E-05	0.000181	2.016	1.991859	0.002016	-0.02414	
Average deviation = 0.000034 Root mean square error = 0.000109 Average absolute = 0.000091								

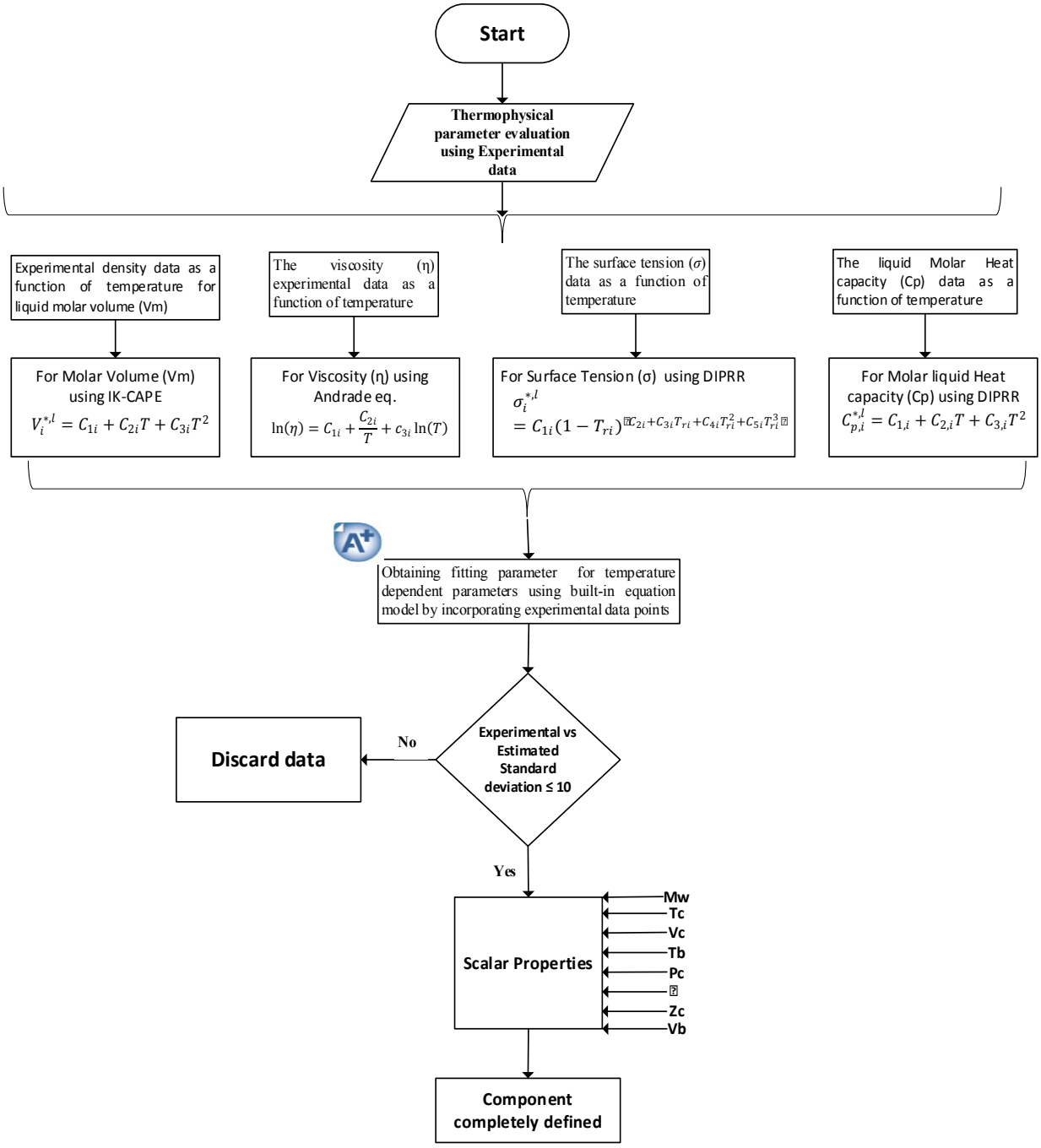

Figure S-1. General procedure for defining component and its properties in Aspen Plus

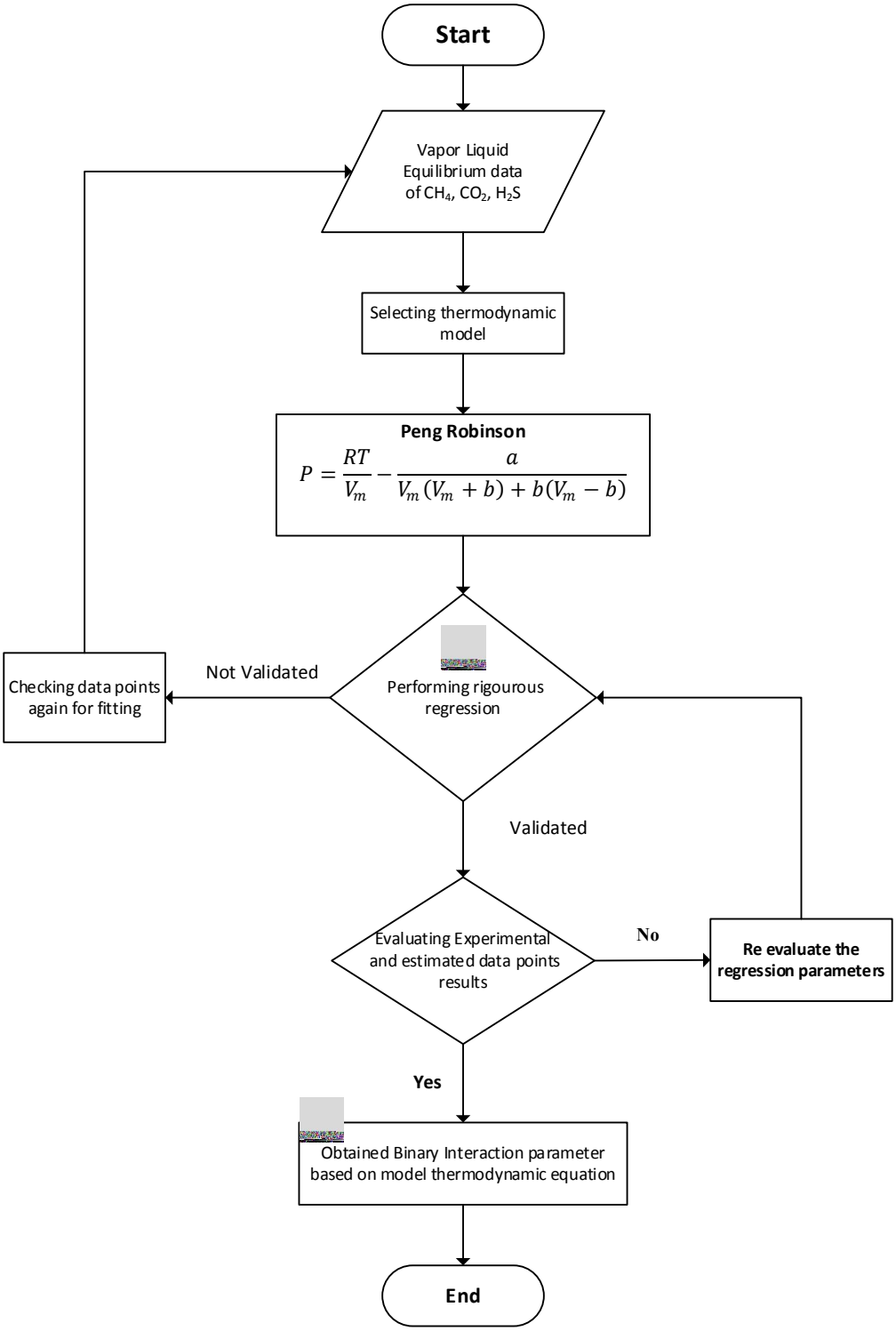

Figure S-2. General procedure of data regression in Aspen Plus

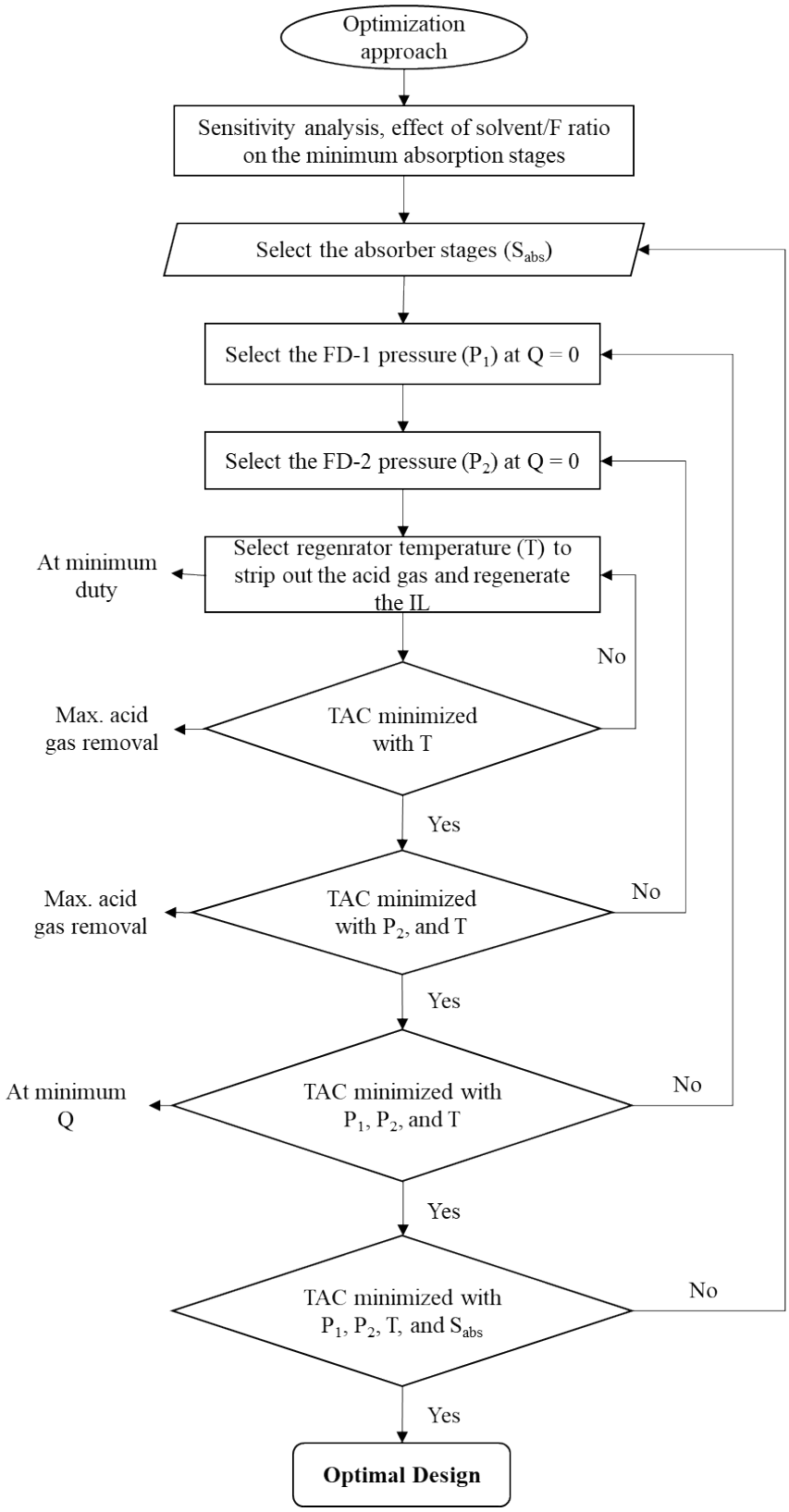

Figure S-3. Process knowledge-based approach for finding optimal design variables

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