Supporting information for Molecular Insight into the Liquid Propan-2-ol + Water Mixture

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Contents

1. Methodology for excess properties

To sample excess properties, three simulations were carried out at a specified pair of temperature and pressure, two for the pure substances and one for the mixture at a specified composition. A binary excess property is then given by

$$y^E = y - x_1 y_1 - x_2 y_2, \tag{1}$$

where y^E represents excess volume v^E or excess enthalpy h^E and x_i are mole fractions. Enthalpy or volume of the two pure substances and their binary mixture are denoted by y_1, y_2 and y, respectively.

In a binary mixture at constant temperature and pressure, partial molar properties $\bar{y}_i$ of each component can be calculated, if the relationship between the molar property and the molar fraction x_i is known

$$\bar{y}_1 = y + x_2 \frac{dy}{dx_1}, \tag{2}$$

$$\bar{y}_2 = y - x_1 \frac{dy}{dx_1}. \tag{3}$$

For that purpose, the Redlich-Kister expression[1] was correlated to present molecular excess property simulation data

$$y^E = x_1 x_2 \sum_{i=1}^{N} A_i (x_1 - x_2)^{i-1}, \tag{4}$$

wherein A_i are fitting parameters.

Employing equations (2) and (3) and the coefficients listed in table 1.1, the resulting partial molar properties at infinite dilution are $v^{\infty}_{\mathrm{H2O}} = 12.51$ cm^3 mol^{-1}, $v^{\infty}_{\mathrm{IPA}} = 65.3$ cm^3 mol^{-1} and $h^{\infty}_{\mathrm{H2O}} = -93.9$ kJ mol^{-1}, $h^{\infty}_{\mathrm{IPA}} = -1.2$ kJ mol^{-1}.

Table 1.1. Coefficients of equation (4).

	A_1	A_2	A_3	A_4	A_5	A_6	A_7	A_8
v^E cm^3 mol^{-1}	-3.287	-1.259	-1.115	-1.958	-1.853			
h^E kJ mol^{-1}	-0.876	2.116	-1.473	0.748	1.080	1.287	-5.147	2.820

2. Molecular simulation details

Monte Carlo and molecular dynamics simulations were carried out with the program ms2[2]. The VLE of pure propan-2-ol was calculated with the grand equilibrium method[3]. Here, the pressure dependence of the chemical potential in the liquid phase was estimated by a first-order Taylor expansion on the basis of simulation results. Subsequently, a molecular simulation run in the pseudo grand canonical ensemble was carried out in order to obtain the saturated vapor phase properties[3]. The second virial coefficient was calculated by integration of Mayer's f function[4]. For the determination of the transport properties, simulations were done in two steps: first, a simulation in the isobaric-isothermal (NpT) ensemble was performed to calculate the density at the desired temperature and pressure. In the second step, a canonic (NVT) ensemble simulation was performed at this temperature and density, to sample the transport properties.

To minimize size and cut-off effects, the simulations were done with 2000 molecules for the pure alcohol and 5000 for the mixture. The simulations in the NpT ensemble were equilibrated over 5×10^5 time steps, followed by a production run over 2×10^7 time steps. In the NVT ensemble, the simulations were equilibrated over 5×10^5 time steps, followed by production runs of 2×10^7 time steps. The self-diffusion coefficient and the shear viscosity were calculated with Eqs. (8) to (10) in the paper employing up to 1×10^5 independent time origins of the autocorrelation functions.

The sampling length of the autocorrelation functions varied between 45 and 60 ps. The separation between the time origins was chosen such that all autocorrelation functions have decayed at least to 1/e of their normalized value to achieve their time independence[5]. The uncertainties of the predicted values were estimated with a block averaging method[6].

To obtain hydrogen bonding statistics, molecular dynamics simulations in the NpT ensemble at 298.15 K and 0.1 MPa containing 2000 molecules in total were carried out. The simulations were equilibrated over 4×10^5 time steps and the production runs had a duration of 10^6 time steps. In all molecular dynamics simulations, Newton's equations of motion were solved using a fifth-order Gear predictor-corrector numerical integrator and the temperature was controlled by velocity scaling. The integration time step was 0.98 fs and the cut-off radius was set to r_c = 17.5 Å. Simulations were carried out in a cubic volume with periodic boundary conditions. The LJ long range interactions were corrected using angle averaging[7]. Electrostatic long-range corrections were considered by the reaction field technique with conducting boundary conditions ($\varepsilon_{RF} = \infty$).

3. Figures

Figure 3.1. Workflow of the present force field parameterization process

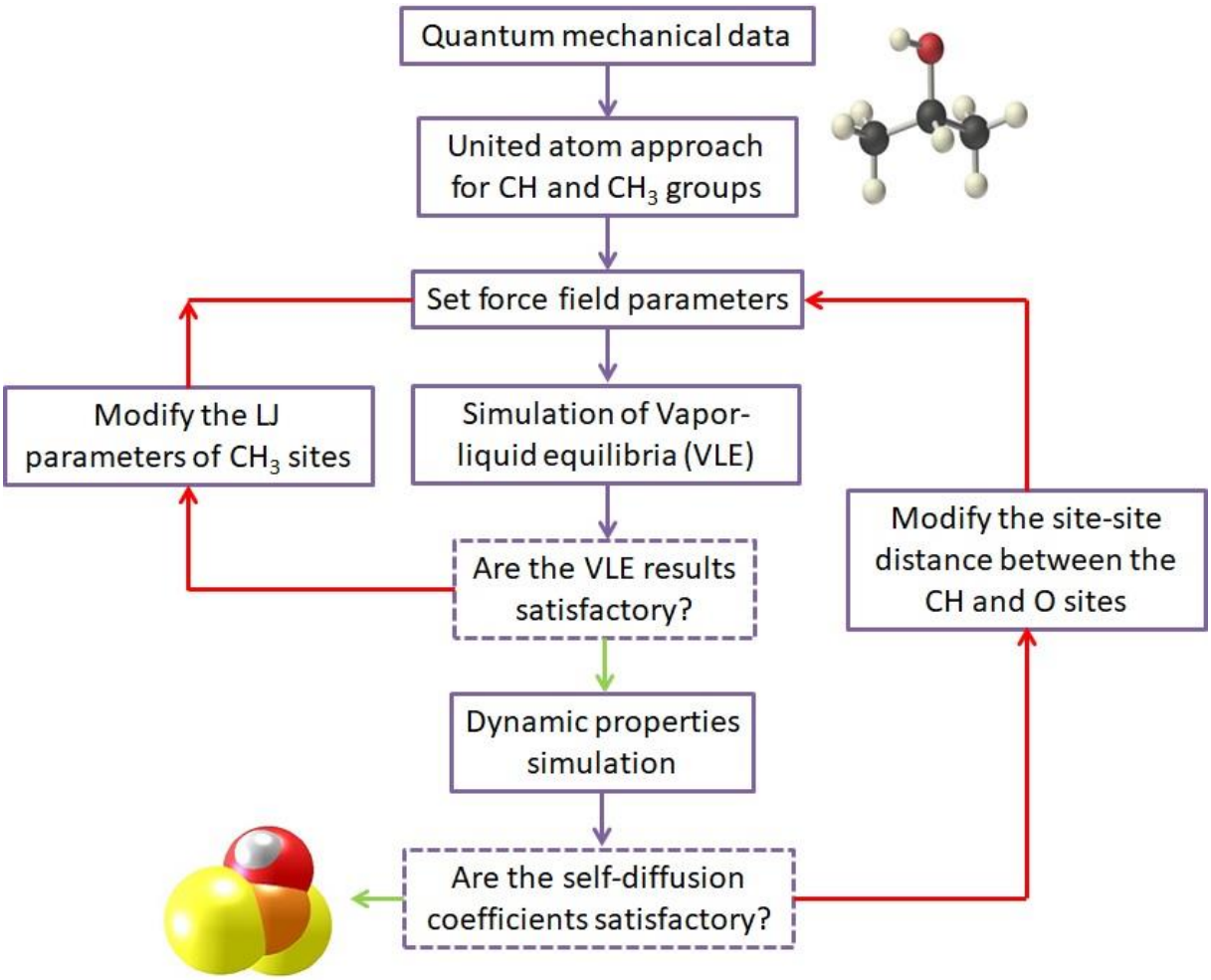


Figure 3.2. Vapor-liquid equilibria of propan-2-ol

Results shown in panels (a), (b), (c) and (d) correspond to the phase envelope, vapor pressure, enthalpy of vaporization and compressibility factor of the vapor phase *z*, respectively. Solid lines represent the DIPPR correlations[8], crosses are experimental data from the literature[9 10 11 12 13 14 15] and squares are molecular simulation results. Blue and white squares are results from the TraPPE-UA[16] and OPLS[17] force fields, respectively. Red squares show results from the present force field.

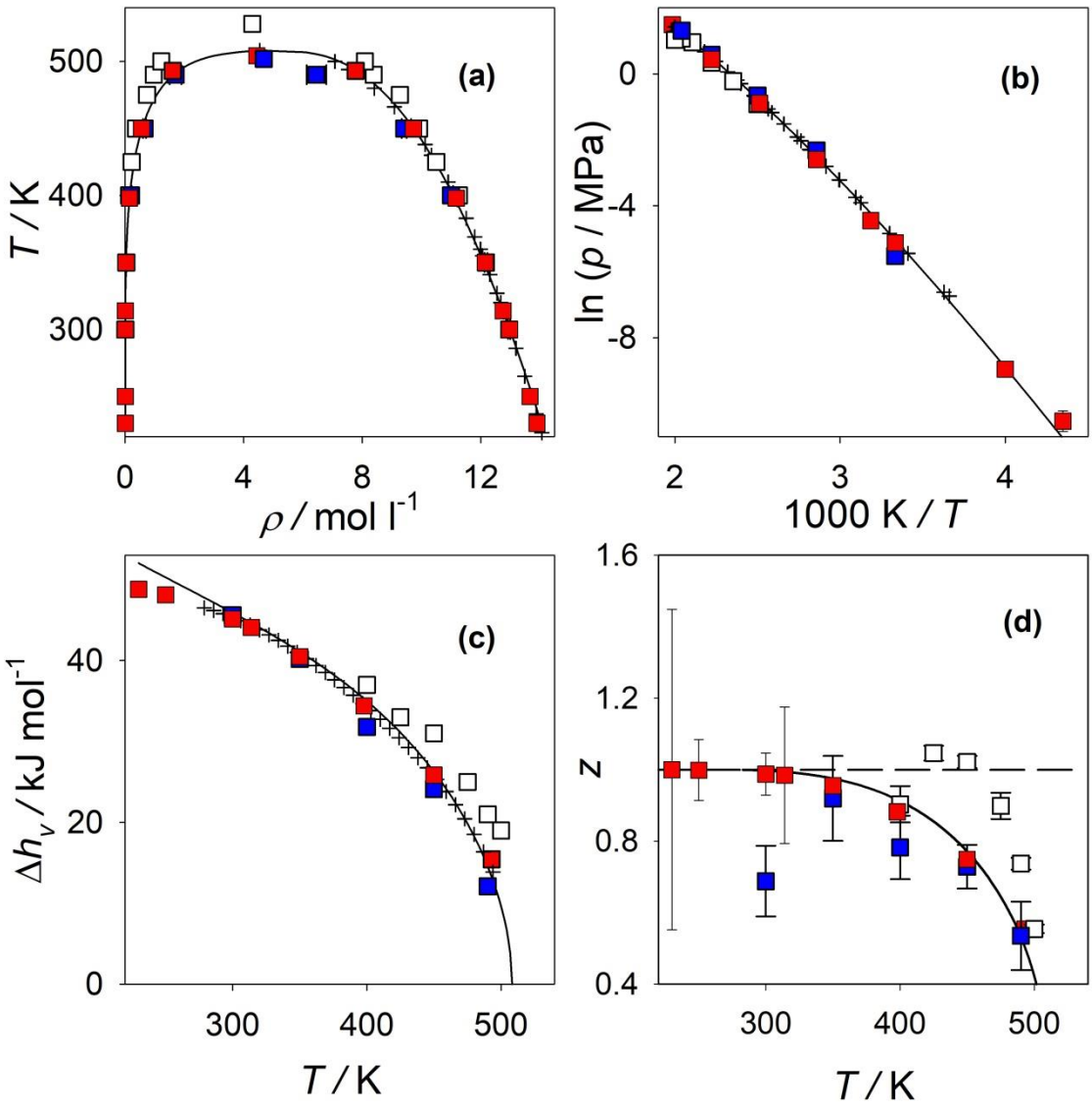


Figure 3.3. Density and self-diffusion coefficient of liquid propan-2-ol at 0.1 MPa

Panels (a), (b) and (c) stand for density, shear viscosity and self-diffusion coefficient. Crosses represent experimental data. White and yellow squares are simulation results by the OPLS all atom force field and the model with optimized partial charges[18]. Red squares show the simulation results with the present force field.

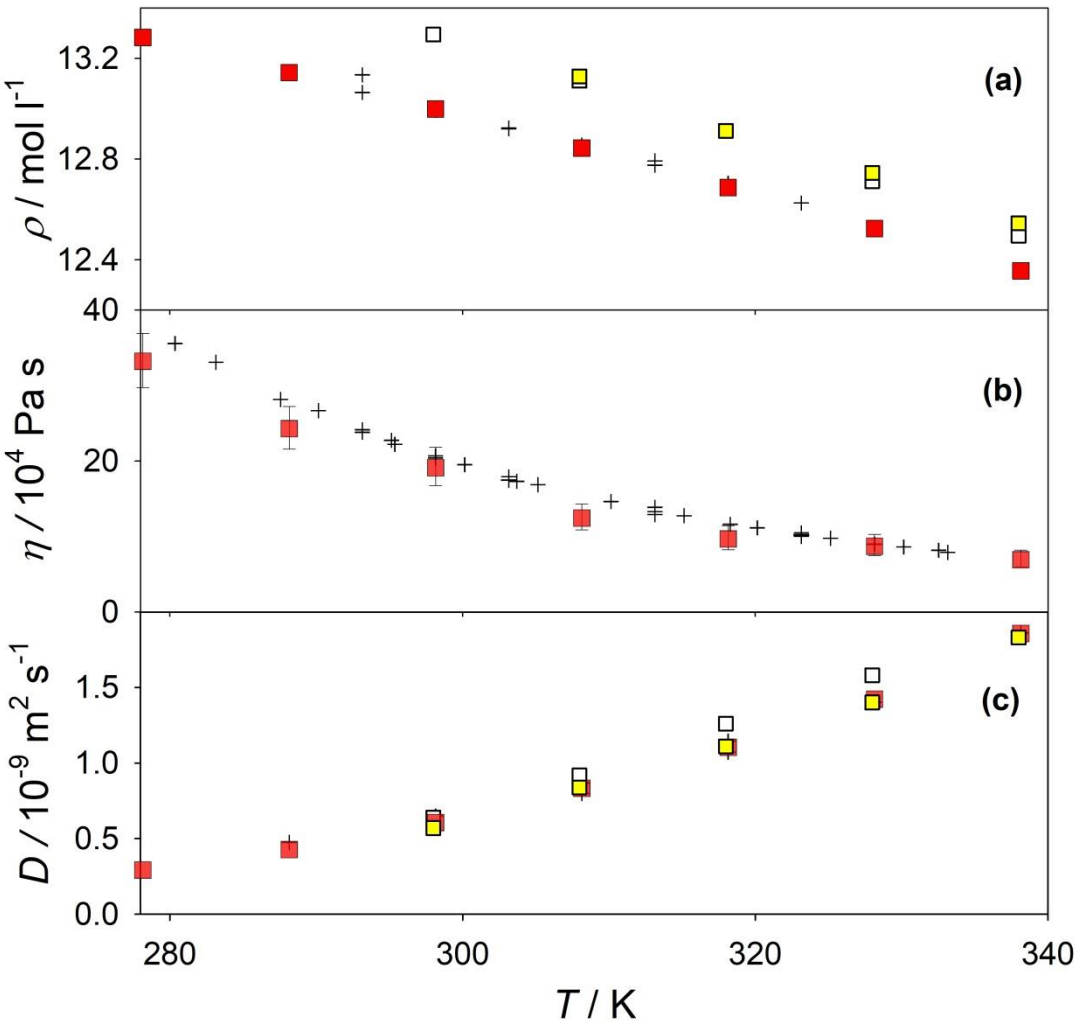


Figure 3.4. Velocity autocorrelation function of propan-2-ol at 298.15 K and 0.1 MPa

The black line represents the VACF and the blue one its running integral.

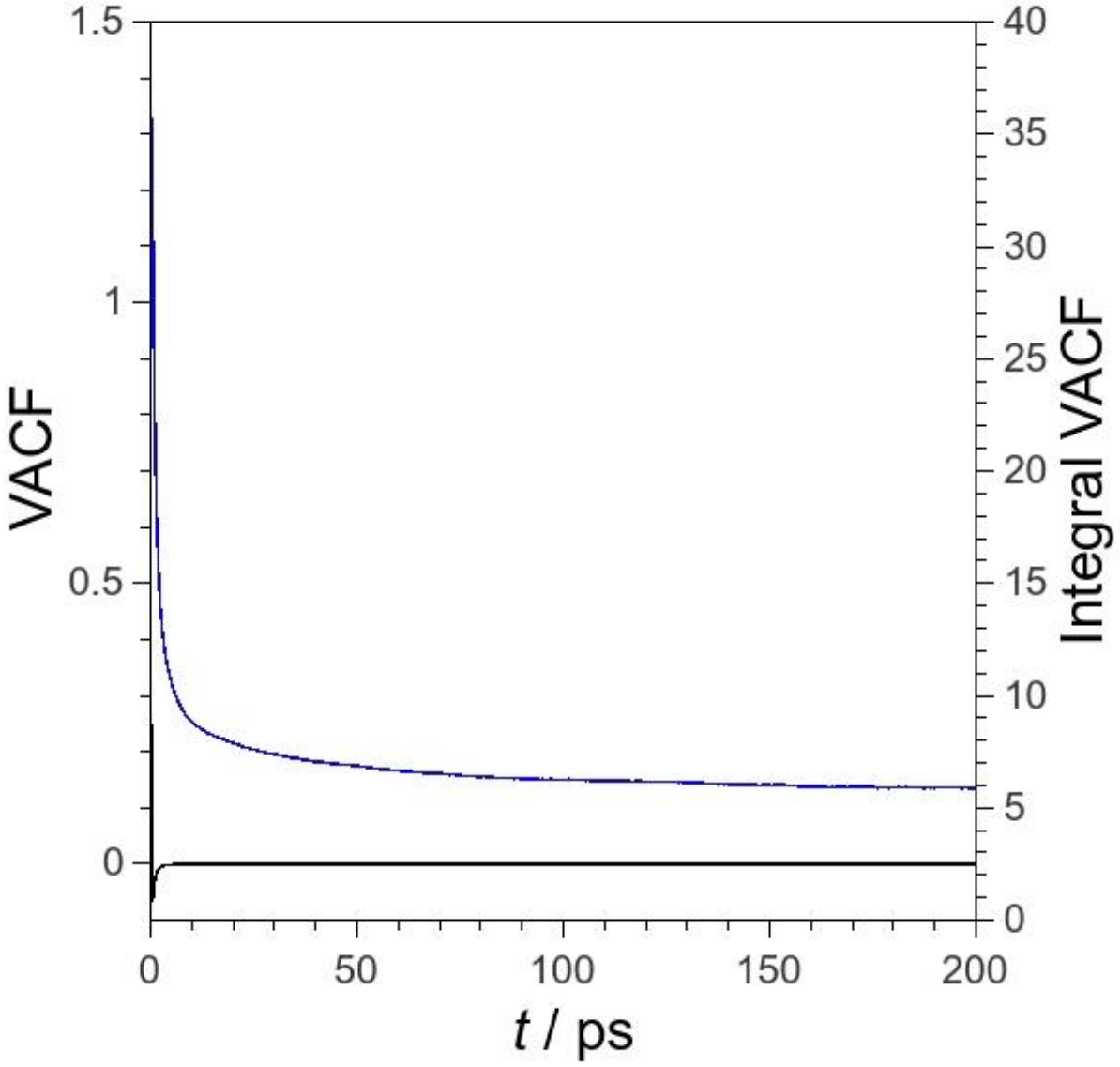


Figure 3.5. Initial decay of the velocity autocorrelation function of propan-2-ol in its mixture with water at 298.15 K and 0.1 MPa

The arrow indicates an increase of the mole fraction of propan-2-ol in the mixture.

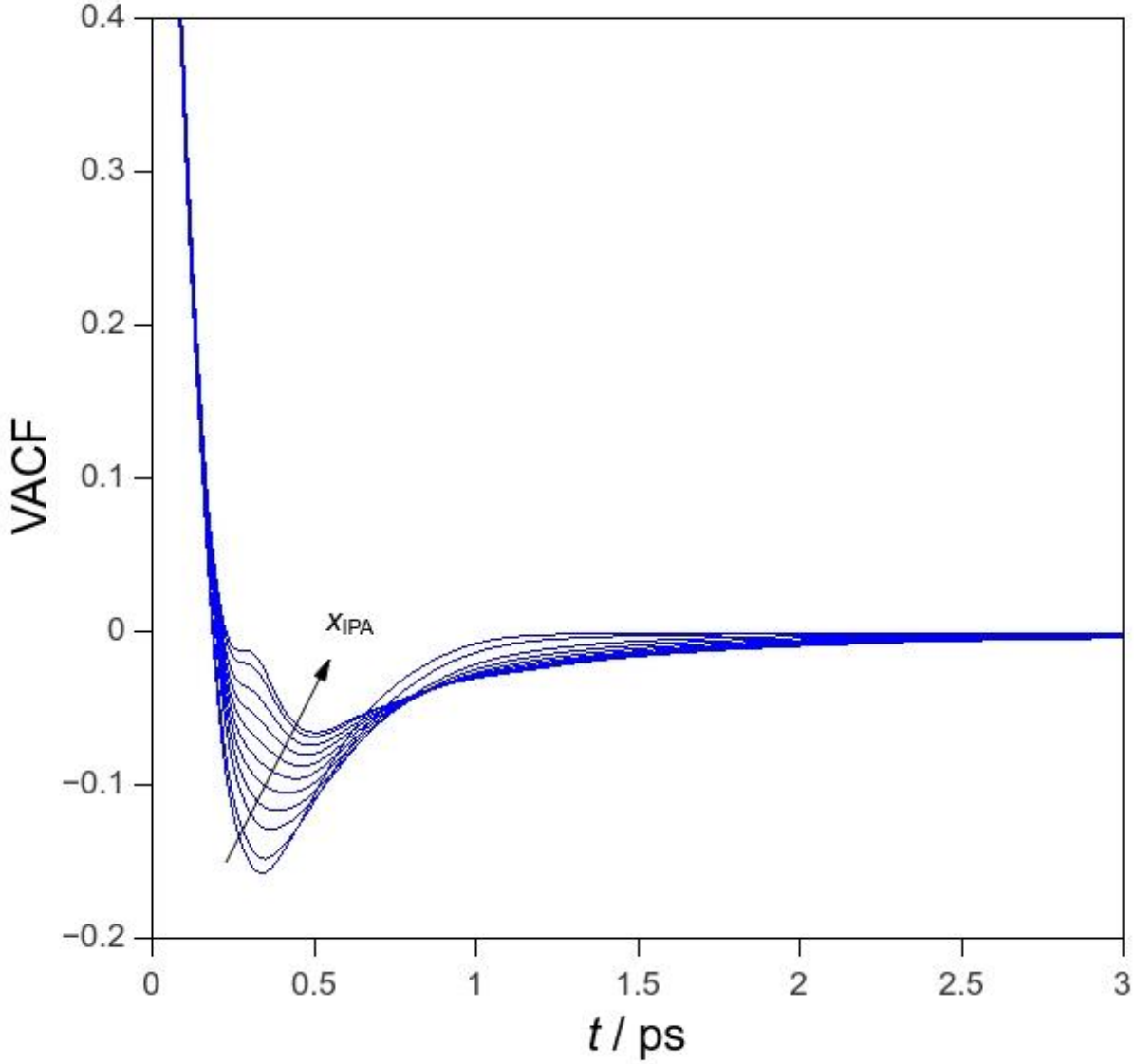
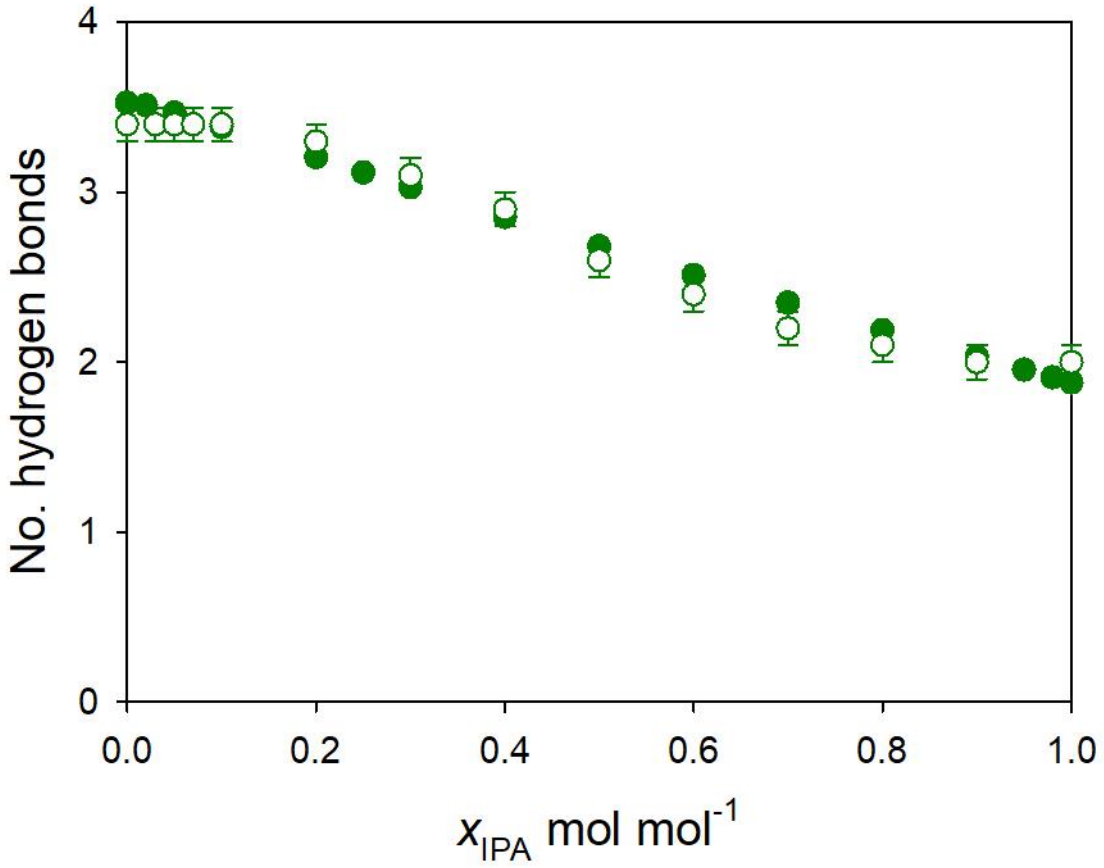


Figure 3.6. Number of hydrogen bonds per oxygen atom as a function of the propan-2-ol mole fraction.

Present molecular simulation results (filled circles) are shown together with literature values based on large-angle X-ray scattering data analysis[19].



4. Tables with simulation results

Table 4.1. Vapor-liquid equilibria of propan-2-ol

Simulation results (sim) on the basis of the present force field are compared to the DIPPR correlations[8]. The number in parentheses indicates the statistical uncertainly in the last digit.

T K	p_{sim} MPa	p_{DIPPR} MPa	$\rho_{L,sim}$ mol l^{-1}	$\rho_{L,DIPPR}$ mol l^{-1}	$\rho_{V,sim}$ mol l^{-1}	$\rho_{V,DIPPR}$ mol l^{-1}	$\Delta h_{v,sim}$ kJ mol^{-1}	$\Delta h_{v,DIPPR}$ kJ mol^{-1}
230	0.000027(8)	0.00002	13.899(3)	14.047	0.000014(4)	0.000008	48.82(1)	52.03
250	0.000129(8)	0.00014	13.666(3)	13.757	0.000062(4)	0.000065	48.11(2)	50.28
300	0.0060(4)	0.0065	12.974(2)	12.980	0.0024(1)	0.0026	45.15(1)	45.92
314	0.012(2)	0.015	12.758(2)	12.746	0.0045(6)	0.0056	44.09(2)	44.64
350	0.075(0)	0.082	12.156(2)	12.104	0.0268(3)	0.0288	40.48(2)	41.09
398	0.409(2)	0.441	11.178(2)	11.117	0.1399(8)	0.1454	34.39(2)	35.29
450	1.544(5)	1.637	9.732(4)	9.735	0.550(2)	0.567	25.84(2)	26.25
483	3.006(8)	3.124	8.35(1)	8.420	1.216(3)	1.318	18.52(4)	17.24
493	3.64(1)	3.72	7.78(2)	7.819	1.602(5)	1.801	15.44(7)	13.27

Table 4.2. Critical point of propan-2-ol

Extrapolated simulation results (sim) from the present force field are compared to recommended data[20] [21], the OPLS[17] and TraPPE-UA[16] results. The number in parentheses indicates the statistical uncertainly in the last digit.

T_c K	p_c MPa	ρ_c mol l^{-1}	Ref.
508.0(6)	4.76(2)		[20]
508.3(3)	4.76(2)	4.51(7)	[21]
528(4)	5(6)	4.3(1)	OPLS [17]
502(2)		4.67(7)	TraPPE-UA[16]
504.24	4.432	4.44	Present

Table 4.3. Second virial coefficient of propan-2-ol

Simulation results (sim) from the present force field are compared to the DIPPR correlation[8],

T K	B_{sim} l mol^{-1}	B_{DIPPR} l mol^{-1}
280	-6.179	-5.651
300	-3.508	-3.268
310	-2.755	-1.263
347	-1.354	-2.569
390	-0.760	-0.735
560	-0.208	-0.225
910	-0.023	0.073
1020	0.000	0.123
1240	0.029	0.196
1520	0.051	0.258
2025	0.010	0.326

Table 4.4. Transport properties of liquid propan-2-ol at 0.1 MPa

The number in parentheses indicates the statistical uncertainly in the last digit. D^{YH} are the self-diffusion coefficient values corrected by the Yeh-Hummer[22] approximation.

T K	ρ mol l^{-1}	D / 10^{-9} m^2 s^{-1}	D^{YH} / 10^{-9} m^2 s^{-}	η / 10^4 Pa s
278.15	13.283	0.282(6)	0.304	33.3(36)
288.15	13.143	0.409(8)	0.438	24.4(28)
298.15	12.999	0.580(8)	0.618	19.3(26)
308.15	12.844	0.786(8)	0.843	12.6(17)
318.15	12.687	1.042(8)	1.114	9.8(16)
328.15	12.524	1.35(1)	1.432	8.9(14)
338.15	12.356	1.77(1)	1.866	7.1(11)

Table 4.5. Liquid structure of propan-2-ol at 0.1 MPa

Oxygen-oxygen and hydrogen-oxygen interactions are represented by $g_{OO}(r)$ and $g_{OH}(r)$, respectively.

T K	ρ mol l^{-1}			*T* K	ρ mol l^{-1}		
278.15	13.302			338.15	12.37		
r Å	$g_{OO}(r)$	$g_{OH}(r)$	ρ(r) mol l^{-1}	*r* Å	$g_{OO}(r)$	$g_{OH}(r)$	ρ(r) mol l^{-1}
0.083	0.000	0.000	0.000	0.085	0.000	0.000	0.000
0.167	0.000	0.000	0.000	0.171	0.000	0.000	0.000
0.250	0.000	0.000	0.000	0.256	0.000	0.000	0.000
0.333	0.000	0.000	0.000	0.341	0.000	0.000	0.000
0.417	0.000	0.000	0.000	0.427	0.000	0.000	0.000
0.500	0.000	0.000	0.000	0.512	0.000	0.000	0.000
0.583	0.000	0.000	0.000	0.597	0.000	0.000	0.000
0.666	0.000	0.000	0.000	0.683	0.000	0.000	0.000
0.750	0.000	0.000	0.000	0.768	0.000	0.000	0.000
0.833	0.000	0.000	0.000	0.853	0.000	0.000	0.000
0.916	0.000	0.000	0.000	0.939	0.000	0.000	0.000
1.000	0.000	0.000	0.000	1.024	0.000	0.000	0.000
1.083	0.000	0.000	0.000	1.109	0.000	0.000	0.000
1.166	0.000	0.000	0.000	1.195	0.000	0.000	0.000
1.250	0.000	0.000	0.000	1.280	0.000	0.000	0.000
1.333	0.000	0.000	0.000	1.365	0.000	0.000	0.000
1.416	0.000	0.000	0.000	1.451	0.000	0.000	0.000
1.499	0.000	0.000	0.000	1.536	0.000	0.008	0.000
1.583	0.000	0.050	0.000	1.621	0.000	0.241	0.000
1.666	0.000	0.858	0.000	1.707	0.000	1.636	0.000
1.749	0.000	3.779	0.000	1.792	0.000	4.174	0.000
1.833	0.000	6.918	0.000	1.878	0.000	5.751	0.000
1.916	0.000	7.288	0.000	1.963	0.000	5.449	0.000
1.999	0.000	5.524	0.000	2.048	0.000	4.162	0.000
2.083	0.000	3.487	0.000	2.134	0.000	2.844	0.000
2.166	0.000	2.013	0.000	2.219	0.000	1.851	0.000
2.249	0.000	1.128	0.000	2.304	0.000	1.198	0.000
2.333	0.000	0.639	0.000	2.390	0.000	0.795	0.000
2.416	0.000	0.377	0.000	2.475	0.003	0.553	0.000
2.499	0.005	0.240	0.000	2.560	0.139	0.424	0.000
2.582	0.243	0.175	0.000	2.646	1.275	0.378	0.000
2.666	2.016	0.164	0.000	2.731	3.779	0.410	0.000
2.749	5.339	0.211	0.000	2.816	5.537	0.530	0.000
2.832	6.855	0.335	0.000	2.902	5.314	0.739	0.000
2.916	5.691	0.550	0.000	2.987	4.024	1.015	0.000
2.999	3.700	0.853	0.000	3.072	2.720	1.321	0.000
3.082	2.139	1.214	0.000	3.158	1.778	1.601	0.000
3.166	1.203	1.571	0.000	3.243	1.188	1.790	0.000
3.249	0.704	1.834	0.000	3.328	0.842	1.835	0.000
3.332	0.456	1.908	0.000	3.414	0.650	1.731	0.005

3.415	0.341	1.766	0.003	3.499	0.548	1.528	0.028
3.499	0.297	1.493	0.023	3.584	0.500	1.311	0.113
3.582	0.290	1.227	0.101	3.670	0.485	1.135	0.335
3.665	0.306	1.040	0.327	3.755	0.491	1.015	0.808
3.749	0.335	0.940	0.853	3.840	0.508	0.940	1.653
3.832	0.372	0.896	1.825	3.926	0.533	0.889	2.932
3.915	0.417	0.877	3.307	4.011	0.565	0.852	4.683
3.999	0.467	0.860	5.266	4.096	0.598	0.815	6.894
4.082	0.522	0.832	7.606	4.182	0.634	0.775	9.493
4.165	0.582	0.788	10.277	4.267	0.672	0.732	12.400
4.248	0.645	0.731	13.246	4.352	0.708	0.688	15.537
4.332	0.710	0.670	16.583	4.438	0.743	0.646	18.645
4.415	0.773	0.612	20.123	4.523	0.773	0.609	21.197
4.498	0.831	0.561	23.331	4.608	0.796	0.580	22.555
4.582	0.877	0.523	25.369	4.694	0.809	0.559	22.463
4.665	0.907	0.499	25.584	4.779	0.812	0.546	21.176
4.748	0.916	0.488	24.100	4.864	0.804	0.540	19.370
4.832	0.905	0.487	21.672	4.950	0.788	0.541	17.666
4.915	0.874	0.494	19.277	5.035	0.765	0.546	16.470
4.998	0.829	0.508	17.550	5.120	0.739	0.555	15.804
5.081	0.777	0.526	16.721	5.206	0.714	0.568	15.586
5.165	0.724	0.547	16.551	5.291	0.693	0.582	15.625
5.248	0.676	0.568	16.748	5.376	0.677	0.598	15.795
5.331	0.639	0.590	17.103	5.462	0.668	0.613	15.994
5.415	0.614	0.611	17.466	5.547	0.667	0.628	16.157
5.498	0.603	0.630	17.736	5.632	0.670	0.643	16.248
5.581	0.604	0.646	17.912	5.718	0.678	0.656	16.265
5.665	0.613	0.660	17.972	5.803	0.687	0.669	16.174
5.748	0.627	0.670	17.892	5.888	0.697	0.682	16.009
5.831	0.644	0.679	17.702	5.974	0.706	0.695	15.763
5.915	0.661	0.689	17.396	6.059	0.716	0.707	15.459
5.998	0.678	0.700	17.015	6.144	0.725	0.720	15.102
6.081	0.694	0.711	16.586	6.230	0.736	0.732	14.709
6.164	0.710	0.723	16.114	6.315	0.747	0.744	14.277
6.248	0.727	0.735	15.623	6.400	0.760	0.756	13.819
6.331	0.744	0.748	15.087	6.486	0.775	0.769	13.321
6.414	0.763	0.761	14.509	6.571	0.790	0.781	12.811
6.498	0.782	0.773	13.923	6.656	0.807	0.793	12.284
6.581	0.803	0.785	13.304	6.742	0.825	0.806	11.752
6.664	0.824	0.798	12.672	6.827	0.843	0.818	11.250
6.748	0.846	0.810	12.041	6.912	0.862	0.831	10.781
6.831	0.867	0.823	11.449	6.998	0.880	0.843	10.362
6.914	0.889	0.837	10.907	7.083	0.899	0.856	10.005
6.997	0.911	0.852	10.418	7.169	0.916	0.870	9.693
7.081	0.930	0.868	9.999	7.254	0.933	0.885	9.456
7.164	0.947	0.884	9.653	7.339	0.948	0.900	9.289
7.247	0.963	0.901	9.406	7.425	0.962	0.915	9.171
7.331	0.977	0.918	9.238	7.510	0.974	0.930	9.119
7.414	0.988	0.935	9.150	7.595	0.986	0.944	9.132

7.497	0.997	0.953	9.149	7.681	0.996	0.959	9.192
7.581	1.006	0.970	9.226	7.766	1.005	0.974	9.305
7.664	1.013	0.986	9.366	7.851	1.013	0.988	9.463
7.747	1.020	1.001	9.572	7.937	1.020	1.001	9.664
7.830	1.027	1.016	9.835	8.022	1.027	1.014	9.898
7.914	1.034	1.029	10.137	8.107	1.031	1.026	10.151
7.997	1.039	1.042	10.480	8.193	1.036	1.037	10.425
8.080	1.045	1.054	10.845	8.278	1.039	1.048	10.708
8.164	1.051	1.065	11.237	8.363	1.041	1.057	10.999
8.247	1.055	1.075	11.628	8.448	1.043	1.065	11.296
8.330	1.058	1.084	12.025	8.534	1.044	1.072	11.586
8.414	1.061	1.092	12.422	8.619	1.045	1.077	11.866
8.497	1.063	1.099	12.796	8.705	1.046	1.082	12.139
8.580	1.065	1.104	13.151	8.790	1.048	1.084	12.392
8.663	1.066	1.107	13.499	8.875	1.050	1.086	12.624
8.747	1.068	1.109	13.803	8.961	1.052	1.087	12.838
8.830	1.070	1.110	14.081	9.046	1.056	1.086	13.028
8.913	1.072	1.110	14.326	9.131	1.059	1.086	13.200
8.997	1.075	1.109	14.535	9.217	1.062	1.086	13.353
9.080	1.077	1.107	14.710	9.302	1.065	1.084	13.480
9.163	1.079	1.105	14.858	9.387	1.068	1.084	13.578
9.247	1.082	1.104	14.966	9.473	1.071	1.082	13.661
9.330	1.085	1.101	15.059	9.558	1.074	1.082	13.724
9.413	1.087	1.099	15.123	9.643	1.076	1.081	13.759
9.496	1.089	1.096	15.151	9.729	1.078	1.080	13.780
9.580	1.090	1.095	15.156	9.814	1.079	1.079	13.774
9.663	1.091	1.093	15.139	9.899	1.080	1.079	13.751
9.746	1.091	1.091	15.104	9.985	1.079	1.078	13.717
9.830	1.091	1.090	15.052	10.070	1.078	1.077	13.673
9.913	1.089	1.088	14.976	10.155	1.077	1.077	13.603
9.996	1.087	1.087	14.881	10.241	1.075	1.076	13.524
10.080	1.085	1.085	14.773	10.326	1.073	1.075	13.437
10.163	1.083	1.083	14.653	10.411	1.071	1.074	13.333
10.246	1.080	1.082	14.512	10.497	1.068	1.073	13.234
10.330	1.076	1.079	14.380	10.582	1.065	1.071	13.125
10.413	1.073	1.077	14.234	10.667	1.062	1.069	13.015
10.496	1.069	1.075	14.086	10.753	1.058	1.066	12.903
10.579	1.065	1.072	13.932	10.838	1.055	1.064	12.786
10.663	1.061	1.069	13.780	10.923	1.051	1.061	12.671
10.746	1.057	1.066	13.643	11.009	1.047	1.058	12.561
10.829	1.052	1.063	13.506	11.094	1.043	1.055	12.460
10.913	1.047	1.059	13.365	11.179	1.039	1.052	12.363
10.996	1.043	1.055	13.238	11.265	1.036	1.048	12.273
11.079	1.038	1.051	13.111	11.350	1.032	1.044	12.191
11.163	1.034	1.046	12.998	11.435	1.028	1.040	12.115
11.246	1.029	1.042	12.895	11.521	1.025	1.036	12.047
11.329	1.025	1.038	12.801	11.606	1.021	1.033	11.986
11.412	1.021	1.033	12.715	11.691	1.019	1.029	11.939
11.496	1.018	1.028	12.645	11.777	1.016	1.025	11.906

11.579	1.014	1.024	12.598	11.862	1.013	1.021	11.877
11.662	1.011	1.019	12.561	11.947	1.011	1.017	11.854
11.746	1.008	1.014	12.535	12.033	1.008	1.014	11.842
11.829	1.005	1.011	12.525	12.118	1.006	1.010	11.834
11.912	1.002	1.006	12.518	12.203	1.004	1.007	11.837
11.996	1.000	1.002	12.527	12.289	1.002	1.004	11.849
12.079	0.998	0.999	12.546	12.374	1.000	1.001	11.866
12.162	0.995	0.995	12.573	12.460	0.997	0.998	11.886
12.245	0.993	0.992	12.606	12.545	0.995	0.996	11.912
12.329	0.991	0.990	12.653	12.630	0.993	0.993	11.943
12.412	0.988	0.987	12.702	12.716	0.991	0.991	11.981
12.495	0.986	0.984	12.752	12.801	0.989	0.989	12.023
12.579	0.984	0.982	12.809	12.886	0.987	0.987	12.063
12.662	0.981	0.980	12.873	12.972	0.985	0.985	12.106
12.745	0.979	0.978	12.936	13.057	0.984	0.983	12.150
12.829	0.978	0.976	13.005	13.142	0.983	0.981	12.195
12.912	0.976	0.974	13.069	13.228	0.981	0.980	12.241
12.995	0.974	0.973	13.135	13.313	0.980	0.978	12.293
13.079	0.973	0.971	13.199	13.398	0.980	0.977	12.330
13.162	0.972	0.970	13.262	13.484	0.979	0.976	12.373
13.245	0.971	0.968	13.330	13.569	0.978	0.975	12.412
13.328	0.970	0.967	13.389	13.654	0.978	0.974	12.449
13.412	0.970	0.966	13.441	13.740	0.978	0.973	12.481
13.495	0.970	0.966	13.488	13.825	0.978	0.973	12.511
13.578	0.970	0.965	13.528	13.910	0.977	0.973	12.543
13.662	0.970	0.965	13.566	13.996	0.977	0.972	12.565
13.745	0.970	0.964	13.600	14.081	0.977	0.972	12.581
13.828	0.970	0.965	13.628	14.166	0.978	0.972	12.597
13.912	0.971	0.965	13.649	14.252	0.978	0.972	12.605
13.995	0.971	0.965	13.661	14.337	0.978	0.973	12.612
14.078	0.972	0.965	13.667	14.422	0.979	0.973	12.609
14.161	0.973	0.966	13.665	14.508	0.979	0.974	12.607
14.245	0.973	0.967	13.659	14.593	0.980	0.974	12.601
14.328	0.974	0.968	13.650	14.678	0.980	0.975	12.591
14.411	0.975	0.969	13.638	14.764	0.981	0.976	12.580
14.495	0.976	0.970	13.622	14.849	0.981	0.977	12.566
14.578	0.977	0.971	13.601	14.934	0.982	0.977	12.551
14.661	0.978	0.972	13.570	15.020	0.983	0.978	12.532
14.745	0.979	0.974	13.541	15.105	0.983	0.979	12.515
14.828	0.980	0.975	13.512	15.190	0.984	0.980	12.492
14.911	0.981	0.977	13.480	15.276	0.985	0.981	12.470
14.994	0.982	0.978	13.445	15.361	0.986	0.982	12.447
15.078	0.983	0.980	13.412	15.446	0.987	0.984	12.423
15.161	0.984	0.981	13.379	15.532	0.987	0.985	12.399
15.244	0.986	0.982	13.344	15.617	0.988	0.986	12.377
15.328	0.987	0.984	13.311	15.702	0.989	0.987	12.355
15.411	0.988	0.985	13.275	15.788	0.990	0.988	12.337
15.494	0.989	0.987	13.248	15.873	0.991	0.989	12.319
15.578	0.990	0.988	13.215	15.958	0.991	0.990	12.306

15.661	0.992	0.990	13.187	16.044	0.992	0.991	12.289
15.744	0.993	0.991	13.166	16.129	0.994	0.993	12.270
15.828	0.994	0.992	13.147	16.214	0.995	0.994	12.256
15.911	0.995	0.994	13.130	16.300	0.996	0.995	12.245
15.994	0.996	0.995	13.115	16.385	0.997	0.996	12.242
16.077	0.997	0.996	13.107	16.470	0.997	0.997	12.241
16.161	0.998	0.998	13.093	16.556	0.998	0.998	12.233
16.244	1.000	0.999	13.089	16.641	0.999	0.999	12.231
16.327	1.000	1.000	13.086	16.726	1.000	1.000	12.232
16.411	1.002	1.002	13.082	16.812	1.001	1.000	12.232
16.494	1.002	1.003	13.087	16.897	1.001	1.001	12.238
16.577	1.003	1.004	13.094	16.982	1.002	1.002	12.243
16.661	1.004	1.005	13.099	17.068	1.003	1.003	12.254
16.744	1.005	1.006	13.114	17.153	1.003	1.004	12.258
16.827	1.006	1.006	13.130	17.238	1.004	1.004	12.268
16.910	1.006	1.007	13.142	17.324	1.004	1.005	12.280
16.994	1.007	1.008	13.161	17.409	1.005	1.006	12.289
17.077	1.008	1.008	13.175	17.495	1.005	1.006	12.300
17.160	1.008	1.009	13.193	17.580	1.006	1.007	12.314
17.244	1.009	1.009	13.213	17.665	1.006	1.007	12.325
17.327	1.009	1.010	13.234	17.751	1.006	1.007	12.337
17.410	1.010	1.010	13.258	17.836	1.006	1.008	12.351
17.494	1.010	1.011	13.275	17.921	1.007	1.008	12.363
17.577	1.009	1.011	13.292	18.007	1.007	1.008	12.376
17.660	1.010	1.011	13.311	18.092	1.007	1.008	12.389
17.743	1.010	1.011	13.326	18.177	1.007	1.008	12.399
17.827	1.010	1.011	13.346	18.263	1.007	1.008	12.409
17.910	1.010	1.011	13.359	18.348	1.007	1.008	12.415
17.993	1.010	1.011	13.376	18.433	1.007	1.008	12.425
18.077	1.010	1.012	13.391	18.519	1.007	1.008	12.430
18.160	1.010	1.011	13.403	18.604	1.007	1.008	12.436
18.243	1.009	1.011	13.412	18.689	1.007	1.008	12.440
18.327	1.009	1.011	13.420	18.775	1.007	1.008	12.445
18.410	1.009	1.011	13.424	18.860	1.007	1.008	12.450
18.493	1.009	1.011	13.429	18.945	1.007	1.008	12.449
18.576	1.009	1.011	13.433	19.031	1.007	1.007	12.451
18.660	1.009	1.010	13.436	19.116	1.007	1.007	12.450
18.743	1.008	1.010	13.435	19.201	1.006	1.007	12.449
18.826	1.008	1.010	13.433	19.287	1.006	1.007	12.445
18.910	1.008	1.009	13.424	19.372	1.006	1.006	12.441
18.993	1.008	1.009	13.419	19.457	1.006	1.006	12.438
19.076	1.007	1.008	13.415	19.543	1.006	1.006	12.434
19.160	1.007	1.008	13.407	19.628	1.005	1.006	12.430
19.243	1.007	1.008	13.399	19.713	1.005	1.006	12.424
19.326	1.007	1.007	13.389	19.799	1.005	1.005	12.419
19.410	1.006	1.007	13.377	19.884	1.004	1.005	12.414
19.493	1.006	1.006	13.369	19.969	1.004	1.005	12.409
19.576	1.006	1.006	13.358	20.055	1.003	1.004	12.400
19.659	1.005	1.005	13.344	20.140	1.003	1.004	12.393

19.743	1.005	1.005	13.331	20.225	1.002	1.004	12.388
19.826	1.004	1.005	13.319	20.311	1.002	1.003	12.382
19.909	1.004	1.004	13.308	20.396	1.002	1.003	12.373
19.993	1.003	1.004	13.299	20.481	1.002	1.003	12.366
20.076	1.003	1.003	13.290	20.567	1.002	1.003	12.360
20.159	1.002	1.003	13.279	20.652	1.001	1.002	12.355
20.243	1.002	1.003	13.272	20.737	1.001	1.002	12.351
20.326	1.001	1.002	13.262	20.823	1.001	1.001	12.350
20.409	1.001	1.002	13.258	20.908	1.001	1.001	12.347
20.492	1.000	1.001	13.251	20.993	1.000	1.001	12.340
20.576	1.000	1.001	13.244	21.079	1.000	1.001	12.339
20.659	1.000	1.000	13.242	21.164	1.000	1.000	12.339
20.742	0.999	1.000	13.238	21.249	1.000	1.000	12.337
20.826	0.999	1.000	13.235	21.335	1.000	1.000	12.340
20.909	0.999	0.999	13.231	21.420	0.999	1.000	12.339
20.992	0.999	0.999	13.232	21.505	0.999	0.999	12.337
21.076	0.998	0.999	13.236	21.591	0.999	0.999	12.336
21.159	0.998	0.998	13.238	21.676	0.999	0.999	12.336
21.242	0.998	0.998	13.238	21.761	0.999	0.999	12.341
21.325	0.998	0.998	13.243	21.847	0.999	0.998	12.345
21.409	0.998	0.997	13.247	21.932	0.998	0.998	12.346
21.492	0.997	0.997	13.255	22.017	0.998	0.998	12.350
21.575	0.997	0.997	13.262	22.103	0.998	0.998	12.352
21.659	0.997	0.997	13.263	22.188	0.998	0.998	12.356
21.742	0.997	0.996	13.270	22.273	0.998	0.998	12.357
21.825	0.997	0.996	13.278	22.359	0.998	0.998	12.360
21.909	0.997	0.994	13.283	22.444	0.998	0.996	12.363
21.992	0.997	0.992	13.290	22.529	0.998	0.995	12.366
22.075	0.997	0.989	13.296	22.615	0.998	0.992	12.367
22.158	0.997	0.985	13.295	22.700	0.998	0.989	12.371
22.242	0.997	0.980	13.302	22.786	0.997	0.985	12.373
22.325	0.997	0.975	13.306	22.871	0.997	0.981	12.374
22.408	0.997	0.969	13.310	22.956	0.998	0.975	12.377
22.492	0.996	0.963	13.314	23.042	0.997	0.969	12.379
22.575	0.993	0.956	13.320	23.127	0.996	0.962	12.382
22.658	0.990	0.948	13.322	23.212	0.994	0.955	12.386
22.742	0.986	0.939	13.326	23.298	0.990	0.946	12.387
22.825	0.981	0.930	13.328	23.383	0.985	0.937	12.387
22.908	0.975	0.920	13.328	23.468	0.980	0.928	12.387
22.992	0.967	0.910	13.331	23.554	0.973	0.917	12.387
23.075	0.959	0.898	13.331	23.639	0.965	0.906	12.386
23.158	0.950	0.887	13.332	23.724	0.956	0.895	12.384
23.241	0.939	0.874	13.334	23.810	0.946	0.882	12.384
23.325	0.928	0.861	13.335	23.895	0.935	0.869	12.386
23.408	0.915	0.847	13.332	23.980	0.923	0.855	12.387
23.491	0.902	0.833	13.330	24.066	0.909	0.841	12.387
23.575	0.888	0.818	13.326	24.151	0.895	0.826	12.383
23.658	0.872	0.802	13.326	24.236	0.880	0.810	12.383
23.741	0.856	0.786	13.323	24.322	0.863	0.793	12.383

23.825	0.839	0.769	13.319	24.407	0.846	0.776	12.381
23.908	0.820	0.752	13.316	24.492	0.828	0.759	12.377
23.991	0.801	0.734	13.315	24.578	0.808	0.740	12.376
24.074	0.781	0.715	13.310	24.663	0.788	0.721	12.372
24.158	0.760	0.695	13.308	24.748	0.767	0.702	12.371
24.241	0.738	0.676	13.307	24.834	0.744	0.681	12.367
24.324	0.715	0.655	13.302	24.919	0.721	0.660	12.367
24.408	0.691	0.634	13.296	25.004	0.697	0.639	12.368
24.491	0.667	0.613	13.294	25.090	0.671	0.617	12.366
24.574	0.641	0.592	13.291	25.175	0.645	0.595	12.363
24.658	0.614	0.571	13.287	25.260	0.618	0.574	12.362
24.741	0.587	0.550	13.284	25.346	0.590	0.553	12.363
24.824	0.558	0.529	13.283	25.431	0.560	0.531	12.363
24.907	0.529	0.509	13.282	25.516	0.530	0.510	12.363
24.991	0.499	0.488	11.453	25.602	0.499	0.489	10.704

Table 4.6. Density ρ, Fick diffusion coefficient D_{12} and shear viscosity η of the liquid binary mixture water + propan-2-ol at 298.15 K and 0.1 MPa as a function of mole fraction

Binary Fick diffusion coefficients indicated with superscript YH correspond to values corrected according to Yeh-Hummer[22]. The number in parentheses indicates the statistical uncertainly in the last digit.

x_{IPA} mol mol^{-1}	ρ mol l^{-1}	D_{12} /10^{-9} m^2 s^{-1}	D_{12}^{YH} /10^{-9} m^2 s^{-1}	η / 10^{-4} Pa s
1	12.996			19.3(16)
0.98	13.210	0.574(60)	0.6143	17.9(7)
0.95	13.539	0.582(80)	0.6207	18.9(9)
0.9	14.122	0.594(90)	0.6330	19.2(6)
0.8	15.450	0.463(80)	0.5006	20.4(7)
0.7	17.042	0.426(62)	0.4610	22.3(8)
0.6	18.987	0.369(50)	0.4030	23.8(9)
0.5	21.417	0.289(44)	0.3225	25.5(8)
0.4	24.540	0.202(38)	0.2347	27.3(12)
0.3	28.675	0.186(38)	0.2167	30.6(14)
0.2	34.415	0.265(34)	0.2993	29.3(14)
0.1	42.812	0.384(47)	0.4292	23.7(10)
0.05	48.431	0.576(87)	0.6395	17.7(10)
0.02	52.316	0.823(105)	0.8881	17.6(7)
0	55.948			17.8(8)

Table 4.7. Intra diffusion coefficient D_i of water and propan-2-ol in their liquid binary mixture at 298.15 K and 0.1 MPa as a function of mole fraction

Intra diffusion coefficients indicated with superscript YH correspond to values corrected according to Yeh-Hummer[22]. The number in parentheses indicates the statistical uncertainly in the last digit.

x_{IPA} mol mol^{-1}	$D_{i,H2O}$ /10^{-9} m^2 s^{-1}	$D_{i,H2O}^{YH}$ /10^{-9} m^2 s^{-1}	$D_{i,IPA}$ /10^{-9} m^2 s^{-1}	$D_{i,IPA}^{YH}$ /10^{-9} m^2 s^{-1}
1			0.580(8)	0.618
0.98	0.593(13)	0.634	0.594(3)	0.634
0.95	0.565(12)	0.603	0.571(3)	0.610
0.9	0.540(10)	0.579	0.565(4)	0.603
0.8	0.509(9)	0.547	0.512(4)	0.550
0.7	0.498(9)	0.534	0.500(4)	0.535
0.6	0.512(8)	0.546	0.476(5)	0.510
0.5	0.574(8)	0.608	0.452(5)	0.485
0.4	0.620(7)	0.652	0.435(6)	0.468
0.3	0.704(6)	0.735	0.420(6)	0.450
0.2	0.816(5)	0.850	0.412(8)	0.446
0.1	1.058(4)	1.103	0.482(8)	0.527
0.05	1.360(3)	1.423	0.613(10)	0.676
0.02	1.779(3)	1.844	0.782(11)	0.847
0	2.155(3)	2.220		

Table 4.8. Average number of hydrogen bonds (AHB) and excess hydrogen bonds (EHB) of the liquid binary mixture at 298.15 K, 0.1 MPa as a function of molar fraction

	AHB of water with		AHB of IPA with		
x_{H2O}	Water	IPA	Water	IPA	EHB
0				1.880	0
0.02	0.107	2.913	0.060	1.828	-0.003
0.05	0.265	2.826	0.150	1.747	-0.006
0.1	0.500	2.599	0.291	1.622	-0.012
0.2	0.956	2.195	0.555	1.392	-0.021
0.25	1.183	2.001	0.676	1.287	-0.024
0.3	1.392	1.821	0.793	1.187	-0.025
0.35	1.606	1.633	0.896	1.101	-0.025
0.4	1.791	1.474	1.003	1.012	-0.024
0.45	1.967	1.323	1.106	0.927	-0.023
0.5	2.138	1.178	1.207	0.844	-0.020
0.6	2.458	0.905	1.397	0.696	-0.014
0.7	2.743	0.664	1.604	0.540	-0.005
0.75	2.876	0.554	1.728	0.448	0.001
0.8	3.016	0.440	1.836	0.371	0.009
0.85	3.145	0.332	1.971	0.290	0.015
0.9	3.278	0.225	2.133	0.190	0.022
0.95	3.408	0.115	2.338	0.091	0.024
0.98	3.490	0.045	2.388	0.041	0.018
1	3.527				0

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