Supporting Information

Thermodynamic and Transport Properties of H_2O+NaCl from Polarizable Force Fields

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Table 1: Force field parameters of BK3 water and ions models.

	Buckingham potential	charge $q(e)$	Gaussian width σ (Å)	polarizability α (A^3)	geometry
H$_2$O	A=322000 kJ/mol B=3.56 Å^{-1} C=3320 kJÅ^6/mol	q_O=-1.168 q_H=0.584	σ_O=0.71 σ_H=0.4	α_O=0.72 α_H=0.36	d_{OH}=0.975Å $\angle$HOH=104.52° d_{OM}=0.2661Å
Na$^+$	A=8.5 $\times$ 10^{12} kJ/mol B=15 Å^{-1} C=550 kJÅ^6/mol	q_{Na} = 11 q_D = -10	σ_{Na}=0.65 σ_D=0.65	α_{Na}=0.157	
Cl$^-$	A=9.4 $\times$ 10^5 kJ/mol B=3.1 Å^{-1} C=8000 kJÅ^6/mol	q_{Cl} = -11 q_D = 10	σ_{Cl}=0.96 σ_D=0.96	α_{Cl}=3.5	

Table 2: Force field parameters of SWM4-NDP water and ions models.

	Lennard-Jones potential	charge $q(e)$	polarizability α (A^3)	geometry
H$_2$O	ϵ=0.883 kJ/mol σ=3.184 Å	q_O=1.71636 q_M=-1.11466 q_H=0.55733 q_D=-1.71636	α_D=0.97825	d_{OH}=0.9572Å $\angle$HOH=104.52° d_{OM}=0.24034Å
Na$^+$	ϵ=0.1316 kJ/mol σ =2.923 Å	q_{Na} = 1.688 q_D = -0.688	α_{Na}=0.157	
Cl$^-$	ϵ=0.3008 kJ/mol σ=4.963 Å	q_{Cl} = 2.46 q_D = -3.46	α_{Cl}=3.969	

Table 3: Force field parameters of SPC/E+SD models

	Lennard-Jones potential	charge q(e)	geometry
H_2O	ϵ=0.65 kJ/mol σ=3.16 Å	q_O=-0.8476 q_M=0.4238	d_{OH}=1.0Å ∠HOH=109.47°
Na^+	ϵ=0.5439 kJ/mol σ=2.35 Å	q_{Na} = 1.0	
Cl^-	ϵ=0.4184 kJ/mol σ=4.4 Å	q_{Cl} = -1.0	

Table 4: Simulation results for relative permittivities ϵ of BK3 and SPC/E water models at T = 298.15 K, 373.15 K and 473.15 K. Statistical uncertainties are given in parentheses in units of the last significant figure shown: 80(2) means 80±2.

T	ϵ	
(K)	BK3	SPC/E
298.15	80(2)	73(2)
373.15	56(2)	53(1)
473.15	34(1)	33(1)

Table 5: Simulation results for the liquid densities ρ (kg/m^3) of BK3 models at T = 298.15 K, 373.15 K, 473.15 K and P = 100 bar. Statistical uncertainties are given as in Table 4.

m	ρ (kg/m^3)		
(mol/kg)	298.15 K	373.15 K	473.15 K
0.00	1002.4(3)	961.9(2)	863.5(2)
0.44	1019.6(3)	978.4(2)	882.8(4)
1.33	1053.5(3)	1010.6(5)	920.3(4)
2.22	1083.1(3)	1037.2(4)	948.3(3)
3.00	1107.2(5)	1060.0(4)	978.5(4)
4.22	1142.5(6)	1093.6(3)	1008.4(4)

Table 6: Simulation results for the liquid densities ρ (kg/m^3) of SPC/E+SD models at T = 298.15 K, 373.15 K, 473.15 K and P = 100 bar. Statistical uncertainties are given as in Table 4.

m	ρ (kg/m^3)		
(mol/kg)	298.15 K	373.15 K	473.15 K
0.00	1001.2(7)	949.1(4)	841(1)
1.00	1040.9(3)	988.4(4)	886.4(6)
2.00	1076.8(3)	1022.6(5)	923.6(6)
3.00	1107.8(5)	1053.1(5)	955.3(6)
4.00	1135.3(3)	1078.2(4)	982.4(5)

Table 7: Simulation results for the electrolyte chemical potential μ (kJ/mol) and mean ionic activity coefficients γ of BK3 models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

m	298.15 K, 1 bar		373.15 K, 1 bar		473.15 K, 15.5 bar	
(mol/kg)	μ (kJ/mol)	$\ln\gamma$	μ (kJ/mol)	$\ln\gamma$	μ (kJ/mol)	$\ln\gamma$
0.11	-409.2(3)	-0.26(1)	-405.6(3)	-0.32(2)	-399.3(4)	-0.46(2)
0.44	-402.8(3)	-0.35(8)	-397.5(3)	-0.39(7)	-389.6(4)	-0.61(7)
1.33	-397.4(3)	-0.41(8)	-391.3(4)	-0.52(7)	-383.2(4)	-0.93(6)
2.22	-394.8(3)	-0.37(8)	-388.0(3)	-0.47(7)	-379.8(4)	-0.98(7)
3.00	-393.1(3)	-0.32(8)	-386.3(3)	-0.51(7)	-378.4(4)	-1.10(7)
4.22	-391.1(3)	-0.26(8)	-384.3(3)	-0.51(7)	-376.5(4)	-1.20(6)

Table 8: Simulation results for the electrolyte chemical potential μ (kJ/mol) and mean ionic activity coefficients γ of SPC/E+SD models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

m	298.15 K, 1 bar [†]		373.15 K, 1bar		473.15 K, 15.5 bar	
(mol/kg)	μ (kJ/mol)	$\ln\gamma$	μ (kJ/mol)	$\ln\gamma$	(mol/kg)	μ (kJ/mol)
0.011	-403.1(2)	-0.138(6)	-400.7(2)	-0.141(4)	-394.0(2)	-0.200(9)
0.06	-395.6(2)	-0.24(5)	–	–	–	–
0.11	–	–	-387.6(2)	-0.33(4)	-378.5(2)	-0.54(3)
0.56	-384.5(2)	-0.31(4)	-378.1(2)	-0.41(4)	-367.6(2)	-0.76(3)
1.00	-381.8(2)	-0.34(4)	-374.0(2)	-0.34(4)	-363.6(2)	-0.85(3)
2.00	-377.7(2)	-0.21(5)	–	–	–	–
3.00	-375.1(2)	-0.10(5)	-367.5(2)	-0.39(4)	-357.0(2)	-1.10(3)
4.00	-373.3(2)	-0.03(5)	–	–	–	–
5.00	-371.7(2)	0.08(5)	-363.9(2)	-0.34(4)	-354.2(2)	-1.25(3)
6.00	-370.5(2)	0.14(5)	-362.9(2)	-0.34(4)	-353.2(2)	-1.32(3)

[†] Data are from Z. Mester and A. Z. Panagiotopoulos, J. Chem. Phys. 142, 044507-10 (2015).

Table 9: Henry's law standard chemical potential $\mu^{†}$ (kJ/mol) of BK3 and SPC/E+SD models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

T(K)	P(bar)	$\mu^{†}_{BK3}$ (kJ/mol)	$\mu^{†}_{SPC/E+SD}$ (kJ/mol)
298.15 K	1.0 bar	-397.0(3)	-380.1(2)
373.15 K	1.0 bar	-389.9(3)	-371.9(2)
473.15 K	15.5 bar	-378.3(4)	-357.0(2)

Table 10: Simulation results for the crystal chemical potential μ (kJ/mol), crystal density ρ (kg/m^3) and salt solubilities of BK3 models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

T (K)	μ (kJ/mol)	ρ (kg/m^3)	solubility (mol/kg)
298.15	-399.0(2)	2115.8(4)	0.99(5)
373.15	-390.6(2)	2097.8(3)	1.48(6)
473.15	-379.4(3)	2073.0(4)	2.5(1)

Table 11: Simulation results for the crystal chemical potential μ (kJ/mol), crystal density ρ (kg/m^3) and salt solubilities of SD models at $T = 298.15$ K, 373.15 K and 473.15 K. Data are from reference [66]. Statistical uncertainties are given as in Table 4.

T (K)	μ (kJ/mol)	ρ (kg/m^3)	solubility (mol/kg)
298.15	-384.019(2)	1932.4(1)	0.63(1)
373.15	-376.241(2)	1916.4(1)	0.73(1)
473.15	-365.331(2)	1894.7(1)	0.78(2)

Table 12: Simulation results for vapor pressures P^{sat} (bar) of BK3 models at $T = 373.15$ K and 473.15 K. Statistical uncertainties are given as in Table 4.

m	P^{sat} (bar)	
(mol/kg)	373.15 K	473.15 K
0.00	1.12(4)†	18.6(4)†
0.43	1.13(4)	18.4(5)
1.30	1.05(4)	18.1(5)
2.17	0.99(5)	17.2(6)
3.03	0.98(4)	16.6(6)
4.33	0.93(5)	16.3(5)
4.99	0.94(7)	16.1(5)

†Data are obtained from extrapolating vapor pressure of solution to zero salt concentration.

Table 13: Fitting parameters in Eq.12 for BK3 models at $T = 373.15$ K and 473.15 K.

Parameter	373.15 K	473.15 K
A	0.604	0.894
B	1.361	1.486
b	-0.216	-0.458
C	0.070	0.099
D	-0.007	-0.008

Table 14: Simulation results for vapor pressures P^{sat} (bar) of AH/SWM4-NDP models at $T = 373.15$ K. Statistical uncertainties are given as in Table 4.

m (mol/kg)	P^{sat} (bar)
0.00	3.1(1)
1.00	3.5(1)
2.00	3.7(1)
3.00	4.0(1)

Table 15: Simulation results for vapor-liquid interfacial tensions σ (mN/m) of BK3 models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

m	σ (mN/m)		
(mol/kg)	298.15 K	373.15 K	473.15 K
0.44	67.9(8)	54.5(8)	33.3(8)
1.33	70(1)	56.8(7)	36.6(6)
2.22	70.5(8)	58.1(6)	39.2(6)
3.00	72(1)	60.3(6)	40.9(6)
4.33	74.0(9)	60.9(7)	42.8(8)
5.00	76.1(7)	62.5(7)	44.2(6)

Table 16: Simulation results for shear viscosities η (cP) of BK3 models at $T = 298.15$ K, 373.15 K and 473.15 K. Statistical uncertainties are given as in Table 4.

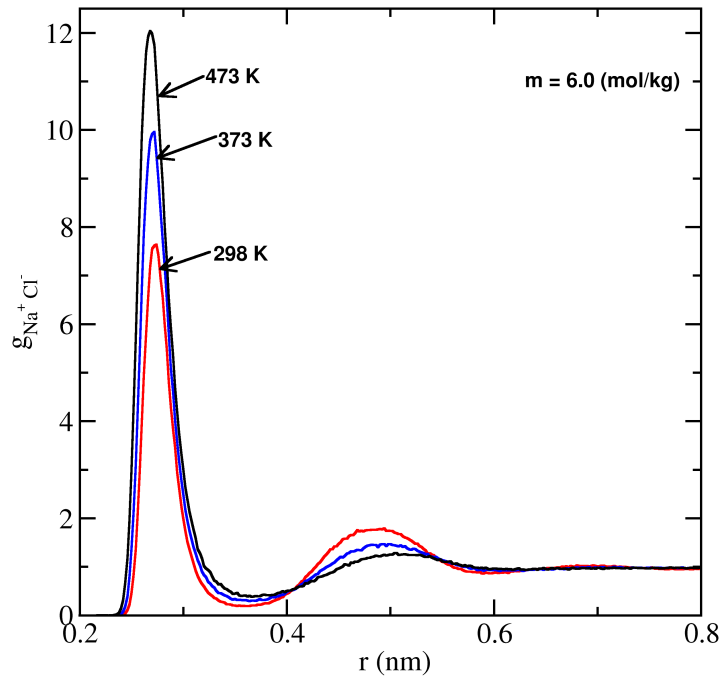| m	η (cP)		
(mol/kg)	298.15 K	373.15 K	473.15 K
0.00	1.00(4)	0.299(8)	0.133(3)
0.44	1.05(1)	0.31(1)	0.145(4)
1.00	1.12(5)	0.33(1)	0.154(2)
2.00	1.29(4)	0.39(1)	0.179(6)
3.00	1.41(3)	0.44(1)	0.199(5)
4.00	1.57(9)	0.51(2)	0.219(4)
6.00	2.4(1)	0.61(2)	0.228(5)

Figure 1: Radial distribution functions between Na^+ and Cl^- of binary H_2O+NaCl mixture with BK3 models at $m = 6.0$, and $T = 298.15$ K, 373.15 K and 473.15 K.
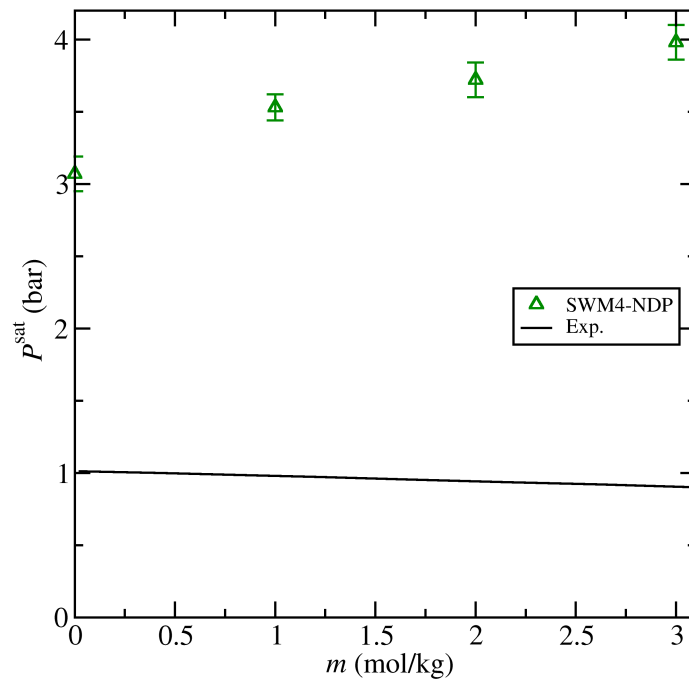
Figure 2: Vapor pressures P^{sat} (bar) for AH/SWM4-NDP models of the system H_2O + NaCl at $T = 373.15$ K *versus* NaCl molality, m, in mol NaCl / kg of H_2O. Symbols are simulation results, and solid line is experimental data (S. L. Phillips, A. Igbene, J. A. Fair, H. Ozbek, and H. Tavana., A Technical Databook for Geothermal Energy Utilization).