

Supplementary material

The NVT-GEMC simulation results for the vapor-liquid equilibrium of water using the SPC-, SPC/E-, and TIP4P-model are summarized in Tables 1 - 3. The NVT-GEMC simulation results for the EPM2-model for carbon dioxide are summarized in Table 4, the NpT-MC results in Table 5. The results of the NpT-GEMC simulations of the binary mixture EPM2-carbon dioxide + TIP4P-water at 348.15 K are summarized in Table 6.

The statistical uncertainties of the results reported in the tables are given in parentheses. For example, the notation 0.017(12) stands for 0.017 ± 0.012 , the notation -8.7(6.3) stands for -8.7 ± 6.3 , and the notation -2078(8) means -2078 ± 8 .

Table 1: VLE data of SPC-H₂O

T / K	N	p / MPa	ρ^I / (g/cm ³)	ρ^{II} / (g/cm ³)	δu^I / (kJ/kg)	δu^{II} / (kJ/kg)
323.15	140	0.017(12)	0.959(6)	0.000071(25)	-2233(8)	-8.7(6.3)
373.15	250	0.106(9)	0.909(5)	0.000664(91)	-2078(8)	-24(11)
423.15	200	0.427(40)	0.843(14)	0.00255(49)	-1916(15)	-40(15)
423.15	200	0.51(11)	0.846(20)	0.00293(61)	-1919(19)	-62(12)
473.15	200	1.62(15)	0.773(9)	0.00883(67)	-1756(5)	-109(24)
473.15	200	1.77(15)	0.772(10)	0.00986(71)	-1751(5)	-170(8)
523.15	200	4.29(45)	0.670(20)	0.0278(45)	-1559(22)	-298(52)
523.15	300	4.76(31)	0.656(18)	0.0263(17)	-1551(16)	-289(31)
553.15	350	7.53(52)	0.558(40)	0.0529(76)	-1393(38)	-434(51)

T / K	δh^I / (kJ/kg)	δh^{II} / (kJ/kg)	Δh^V / (kJ/kg)
323.15	-2382(8)	83(189)	2465(189)
373.15	-2250(8)	-37(28)	2213(29)
423.15	-2110(15)	-68(39)	2043(41)
423.15	-2114(19)	-82(53)	2032(56)
473.15	-1972(5)	-144(32)	1828(33)
473.15	-1968(5)	-209(21)	1759(22)
523.15	-1794(22)	-385(60)	1409(64)
523.15	-1785(16)	-350(35)	1435(38)
553.15	-1635(38)	-547(55)	1088(67)

Table 2: VLE data of SPC/E-H₂O

T / K	N	p / MPa	ρ^I / (g/cm ³)	ρ^{II} / (g/cm ³)	δu^I / (kJ/kg)	δu^{II} / (kJ/kg)
323.15	140	0.002(2)	0.989(7)	0.000040(37)	-2515(6)	-3.1(3.6)
373.15	200	0.035(4)	0.943(8)	0.000226(68)	-2347(19)	-19(17)
423.15	300	0.217(12)	0.886(3)	0.001169(99)	-2185(4)	-26(11)
473.15	300	0.823(59)	0.830(8)	0.00398(34)	-2017(12)	-68(24)
523.15	300	2.58(22)	0.758(7)	0.01407(82)	-1851(11)	-247(37)
573.15	200	5.50(56)	0.620(42)	0.0300(41)	-1620(43)	-324(52)
573.15	350	5.36(33)	0.622(23)	0.0297(34)	-1623(23)	-338(64)

T / K	δh^I / (kJ/kg)	δh^{II} / (kJ/kg)	Δh^V / (kJ/kg)
323.15	-2664(6)	-92(68)	2572(68)
373.15	-2519(19)	-34(53)	2485(56)
423.15	-2380(4)	-35(22)	2345(22)
473.15	-2234(12)	-80(33)	2154(35)
523.15	-2089(11)	-306(41)	1783(42)
573.15	-1876(43)	-405(60)	1471(74)
573.15	-1878(23)	-422(68)	1456(72)

Table 3: VLE data of TIP4P-H₂O

T / K	N	p / MPa	$\rho^I / (\text{g/cm}^3)$	$\rho^{II} / (\text{g/cm}^3)$	$\delta u^I / (\text{kJ/kg})$	$\delta u^{II} / (\text{kJ/kg})$
323.15	200	0.0183(26)	0.981(6)	0.000123(25)	-2216(8)	-1.3(2.1)
373.15	200	0.155(26)	0.926(13)	0.00089(16)	-2045(13)	-37(18)
423.15	200	0.658(20)	0.865(7)	0.00363(21)	-1877(9)	-59(25)
473.15	200	2.19(25)	0.791(7)	0.0128(15)	-1706(8)	-189(35)
523.15	250	5.36(64)	0.672(16)	0.0289(23)	-1504(17)	-256(17)
553.15	250	9.07(36)	0.564(15)	0.0584(57)	-1339(13)	-422(36)
573.15	300	12.5(1.1)	0.377(18)	0.106(17)	-1101(25)	-576(59)

T / K	$\delta h^I / (\text{kJ/kg})$	$\delta h^{II} / (\text{kJ/kg})$	$\Delta h^V / (\text{kJ/kg})$
323.15	-2365(8)	-1(37)	2364(38)
373.15	-2217(13)	-34(47)	2183(49)
423.15	-2072(9)	-74(28)	1998(29)
473.15	-1921(8)	-236(45)	1685(45)
523.15	-1738(17)	-312(31)	1426(35)
553.15	-1579(13)	-522(40)	1056(42)
573.15	-1324(26)	-713(63)	610(67)

Table 4: VLE data of EPM2-CO₂

T / K	N	p / MPa	ρ^I / (g/cm ³)	ρ^{II} / (g/cm ³)	δu^I / (kJ/kg)	δu^{II} / (kJ/kg)
230.15	250	1.02(19)	1.123(3)	0.0273(43)	-295(1)	-9.4(1.7)
240.15	250	1.46(19)	1.078(10)	0.0332(36)	-280(3)	-11.7(1.5)
250.15	250	1.83(14)	1.031(9)	0.0457(29)	-264(3)	-15.9(1.3)
250.15	300	1.93(6)	1.034(10)	0.0492(33)	-265(3)	-17.8(1.4)
260.15	250	2.66(21)	0.985(3)	0.0662(47)	-250(1)	-22.3(1.8)
270.15	250	3.30(17)	0.929(5)	0.0871(45)	-233(1)	-28.1(1.5)
280.15	300	4.30(18)	0.854(22)	0.112(10)	-212(5)	-34.9(3.3)
285.15	250	5.04(27)	0.824(31)	0.140(13)	-204(8)	-42.4(4.5)
290.15	350	5.67(26)	0.778(10)	0.157(11)	-193(2)	-46.6(2.8)

T / K	δh^I / (kJ/kg)	δh^{II} / (kJ/kg)	Δh^V / (kJ/kg)
230.15	-338(1)	-15(9)	323(9)
240.15	-324(3)	-13(8)	310(8)
250.15	-310(3)	-23(4)	287(5)
250.15	-311(3)	-26(3)	285(5)
260.15	-296(1)	-31(5)	265(5)
270.15	-280(1)	-41(3)	239(3)
280.15	-260(5)	-50(5)	211(7)
285.15	-252(8)	-60(6)	191(10)
290.15	-240(2)	-65(4)	175(4)

Table 5: EPM2-CO₂ at supercritical conditions

T / K	p / MPa	N	ρ / (g/cm ³)	u / (kJ/kg)	h / (kJ/kg)
310.0	5.0	250	0.110(2)	-31.9(3)	-45.1(7)
310.0	10.0	250	0.602(74)	-150(16)	-192(16)
310.0	10.0	50	0.5(1)	-124(22)	-162(23)
310.0	10.0	250	0.642(28)	-158(5)	-201(5)
310.0	20.0	250	0.832(6)	-200(2)	-234(2)
310.0	30.0	250	0.910(16)	-219(5)	-245(5)
310.0	40.0	250	0.947(9)	-229(2)	-245(2)
310.0	50.0	250	0.980(8)	-237(2)	-244(2)
310.0	60.0	250	1.010(11)	-244(3)	-243(3)
310.0	70.0	250	1.037(5)	-252(2)	-243(2)
320.0	5.0	250	0.103(1)	-28.9(2)	-40.7(6)
320.0	10.0	250	0.337(17)	-89.0(4.0)	-120(4)
320.0	10.0	50	0.336(35)	-86.5(7.4)	-117(8)
320.0	10.0	250	0.321(23)	-85.6(6.2)	-115(7)
320.0	10.0	50	0.312(24)	-80.2(5.8)	-109(6)
320.0	20.0	250	0.785(20)	-188(4)	-223(5)
320.0	30.0	250	0.861(21)	-206(5)	-231(5)
320.0	40.0	250	0.918(8)	-219(3)	-236(3)
320.0	50.0	250	0.950(9)	-228(2)	-236(2)
320.0	60.0	250	0.985(9)	-236(2)	-236(2)
320.0	70.0	250	1.012(6)	-243(2)	-234(2)

Table 5: EPM2-CO₂ at supercritical conditions (continued)

T / K	p / MPa	N	ρ / (g/cm ³)	u / (kJ/kg)	h / (kJ/kg)
350.0	2.5	250	0.0405(1)	-10.5(1)	-14.8(2)
350.0	5.0	250	0.0878(9)	-22.9(2)	-32.1(6)
350.0	10.0	250	0.215(5)	-54.9(1.0)	-74.5(1.4)
350.0	20.0	250	0.576(10)	-136(2)	-167(2)
350.0	20.0	50	0.601(35)	-140(7)	-172(8)
350.0	30.0	250	0.730(13)	-169(3)	-194(3)
390.0	2.5	250	0.0355(2)	-8.4(1)	-11.8(3)
390.0	5.0	250	0.0743(5)	-18.0(1)	-24.4(4)
390.0	10.0	250	0.165(2)	-39.7(7)	-52.7(1.1)
390.0	20.0	250	0.388(6)	-89.6(1.6)	-112(2)
390.0	30.0	250	0.574(18)	-129(3)	-151(4)
520.0	2.5	250	0.0258(2)	-5.00(5)	-6.3(6)
520.0	5.0	250	0.0522(4)	-10.6(1)	-13.1(8)
520.0	10.0	250	0.1060(6)	-21.8(2)	-25.7(6)
520.0	20.0	250	0.2155(8)	-44.4(2)	-49.8(4)
520.0	30.0	250	0.319(2)	-65.4(4)	-69.7(7)
520.0	50.0	250	0.486(4)	-99.3(7)	-94.8(1.1)

Table 6: Simulation results for the binary mixture CO₂-H₂O using the EPM2-model and the TIP4P-model at 348.15 K

p / MPa	N	$\rho^I / (\text{g/cm}^3)$	$\rho^{II} / (\text{g/cm}^3)$	$u^I / (\text{kJ/kg})$	$u^{II} / (\text{kJ/kg})$	x_{CO_2}	y_{CO_2}
5.033	300	0.954(5)	0.0877(22)	-2079(17)	-23.0(0.5)	0.0102(42)	0.9891(2)
7.500	450	0.959(8)	0.1421(23)	-2083(13)	-37.7(0.7)	0.0106(22)	0.9907(22)
7.599	300	0.957(7)	0.1479(41)	-2059(22)	-38.5(1.1)	0.0140(41)	0.9922(14)
10.000	450	0.964(6)	0.2143(76)	-2077(14)	-55.5(2.1)	0.0111(22)	0.9920(10)
10.132	300	0.968(9)	0.222(10)	-2070(25)	-57.1(2.5)	0.0122(36)	0.9919(26)
12.665	300	0.964(8)	0.311(18)	-2066(21)	-78.0(3.9)	0.0129(26)	0.9932(14)