Modelling of hydrate dissociation curves with a modified Cubic-Plus-Association equation of state.

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Supporting information

Table A1 – Gas mixtures feed compositions.

	wt %								
mixture	CH_4	C_2H_6	C_3H_8	C_4H_{10}	iC_4H_{10}	C_5H_{12}	N_2	CO_2	H_2S
Sour gas 1 [1]	65.8	0.00	0.00	0.00	0.00	0.00	4.18	24.08	5.92
Sour gas 2 [1]	52.6	0.00	0.00	0.00	0.00	0.00	2.50	34.33	10.57
Sour gas 3 [1]	71.0	0.00	0.00	0.00	0.00	0.00	0.73	11.48	16.80
Natural gas 1 [2]	86.5	7.45	4.11	0.00	0.00	0.00	0.70	1.23	0.00
Natural gas 2 [3]	79.5	10.62	6.59	1.57	1.54	0.08	0.06	0.00	0.00
Natural gas 3 [4]	63.2	15.20	10.80	2.05	4.70	0.00	0.15	3.92	0.00
CH_4+C_2H_6+N_2+CO_2 [5]	78.8	8.46	0.00	0.00	0.00	0.00	0.03	12.67	0.00
CH_4+C_3H_8+N_2+CO_2 [5]	75.5	0.00	5.78	0.00	0.00	0.00	0.03	18.73	0.00
CH_4+N_2+CO_2 [5]	91.5	0.00	0.00	0.00	0.00	0.00	0.08	8.39	0.00
CH_4+C_2H_6+N_2 [5]	84.7	8.53	0.00	0.00	0.00	0.00	6.80	0.00	0.00

Table A2 – *%AAD* on composition for mixtures of $H_2O + CO_2 + CH_4$. Data from Belandria *et al.* [6]

Feed (mol)						***%AAD* CO_2**		***%AAD* aqueous phase**	
water	methane	CO2	T/K	P/Mpa	gas	hydrate	water	methane	water
1.43	0.165	0.048	273.6	2.234	30.6	a)	a)	a)	a)
5.236	0.165	0.048	273.6	2.416	10.6	a)	a)	a)	a)
8.185	0.165	0.048	273.6	2.440	27.4	118.2	61.9	42.6	0.3
1.65	0.115	0.116	273.6	1.844	15.3	6.7	35.1	53.1	0.3
5.355	0.115	0.116	273.6	1.941	16.4	33.4	8.9	11.9	0.1
8.48	0.115	0.116	273.6	2.048	24.6	54.6	49.2	100.7	0.4
1.696	0.057	0.181	273.6	1.510	9.3	7.7	25.7	102.6	0.3
5.182	0.057	0.181	273.6	1.607	8.1	6.8	33.6	180.7	0.4
1.43	0.165	0.048	275.2	2.583	21.3	5.4	41.7	1.1	0.3
5.236	0.165	0.048	275.2	2.712	18.5	a)	a)	a)	a)
8.185	0.165	0.048	275.2	2.766	55.0	b)	b)	b)	b)
1.65	0.115	0.116	275.2	2.123	13.0	5.6	29.4	60.9	0.3
5.355	0.115	0.116	275.2	2.220	24.3	4.8	8.9	8.2	0.1
8.48	0.115	0.116	275.2	2.400	23.3	24.8	49.6	124.3	0.5
1.696	0.057	0.181	275.2	1.792	5.6	1.9	13.4	14.9	0.2
5.182	0.057	0.181	275.2	1.865	10.9	2.3	12.1	3.9	0.1
1.43	0.165	0.048	276.1	2.813	13.4	b)	b)	b)	b)
5.236	0.165	0.048	276.1	3.025	1.1	7.4	9.1	6.9	0.0
8.185	0.165	0.048	276.1	3.027	35.8	b)	b)	b)	b)
1.65	0.115	0.116	276.1	2.318	10.0	3.7	27.0	26.8	0.3
5.355	0.115	0.116	276.1	2.503	9.1	30.5	40.2	58.8	0.4
8.48	0.115	0.116	276.1	2.690	11.1	36.4	52.5	89.4	0.6
1.696	0.057	0.181	276.1	1.985	2.9	7.7	28.4	27.1	0.5
5.182	0.057	0.181	276.1	2.174	c)	8.3	13.9	5.9	0.2
1.43	0.165	0.048	278.1	3.416	0.7	b)	b)	b)	b)
5.236	0.165	0.048	278.1	3.631	8.1	b)	b)	b)	b)
8.185	0.165	0.048	278.1	3.802	8.4	43.6	57.3	45.5	0.4
5.355	0.115	0.116	278.1	3.037	14.7	18.4	34.3	76.9	0.4
8.48	0.115	0.116	278.1	3.319	10.6	52.8	52.0	121.6	0.6
1.696	0.057	0.181	278.1	2.450	3.2	a)	a)	a)	a)
5.182	0.057	0.181	278.1	2.580	2.2	3.9	11.3	4.7	0.2
1.43	0.165	0.048	279.2	3.565	0.7	b)	b)	b)	b)
5.236	0.165	0.048	280.2	4.486	1.7	b)	b)	b)	b)
8.185	0.165	0.048	280.2	4.655	8.3	b)	b)	b)	b)
5.355	0.115	0.116	280.2	3.541	10.2	b)	b)	b)	b)
8.48	0.115	0.116	280.2	4.109	16.6	1.6	36.8	103.1	0.4
5.182	0.057	0.181	280.2	3.139	6.1	b)	b)	b)	b)
8.395	0.057	0.181	280.2	3.481	6.4	15.4	18.4	204.3	0.2
8.185	0.165	0.048	282.2	5.767	2.5	b)	b)	b)	b)
8.185	0.165	0.048	284.2	7.190	7.8	b)	b)	b)	b)
				Averages	13.0	20.9	31.3	61.5	0.3

a) CPA predicts liquid and hydrate phases, which were not experimentally verified. b) CPA only predicts a gas phase when the experimental data is triphasic. c) CPA does not present a gas phase.

Table A3 – Obtained ΔT between the experimental data on hydrate the hydrate composition data and the CPA results. Data from Ng. [7]

mixture	P/MPa	T_{exp}/K	$\Delta T_{(exp\text{-}model)}$/K
1	2.07	284.55	0.00
1	6.89	293.25	0.00
2	2.07	276.85	0.05
2	6.89	286.35	0.00
3	2.07	284.05	0.35
3	6.89	292.55	0.00
4	2.07	286.05	1.06
4	6.89	294.75	0.75
5	2.07	284.45	0.41
5	6.89	292.75	0.00
6	2.07	282.95	0.39
6	6.89	291.85	0.00

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