Supporting information

Modelling hydrate dissociation curves in the presence of hydrate inhibitors with a modified CPA EoS.

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Table S1 – Absolute average deviations (%) for pressures, in Pa, of the systems water with methanol, ethanol.

water : methanol				water : ethanol			
T/K	Ref.	Pbub	Pdew	T/K	Ref.	Pbub	Pdew
323	[1]	2.37	0.98	298	[2]	3.36	2.59
328	[1]	2.60	1.22	313	[3]	6.09	0.88
333	[1]	3.04	2.13	363	[4]	1.40	4.18
363	[5]	4.85		381	[4]	1.65	2.73
383	[5]	3.86		403	[4]	2.91	2.69
403	[5]	5.30		423	[4]	2.43	1.51
424	[5]	2.75		473	[6]	0.75	
442	[5]	6.53		473	[7]	2.31	1.46
				523	[6]	1.12	
				523	[7]	0.97	0.62
				548	[6]	0.49	
				548	[7]	1.59	0.59
				573	[6]	1.83	0.99

Table S2 – Absolute average deviations (%) on mole fractions of the systems water with methanol, ethanol.

water : methanol				water : ethanol			
T/K	Ref.	y_1	x_1	T/K	Ref.	y_1	x_1
323	[1]	4.21	3.74	298	[2]	9.20	14.03
328	[1]	4.89	4.23	313	[3]	9.48	5.96
333	[1]	5.19	4.14	363	[4]	10.63	14.52
				381	[4]	10.87	12.63
				403	[4]	14.06	11.17
				423	[4]	6.44	5.62
				473	[6]	2.10	1.79
				523	[6]	1.00	0.86
				548	[6]	0.93	1.37
				573	[6]	1.41	1.04

Table S3 – Compositions of the gases on section 3.3 of this work.

Gas/ Compound	**% mol**				
	mixture 1[8]	natural gas[9]	sour gas 1[10]	sour gas 2[10]	sour gas 3[10]
N_2	0	0.04	3.00	2.00	0.50
H_2S	0	0	3.49	6.96	9.47
CO_2	0	0	11.00	17.50	5.01
methane	91.00	89.86	82.51	73.54	85.02
ethane	9.00	6.40	0	0	0
propane	0	2.71	0	0	0
iso-butane	0	0.48	0	0	0
n-butane	0	0.49	0	0	0
iso-pentane	0	0	0	0	0
n-pentane	0	0.02	0	0	0

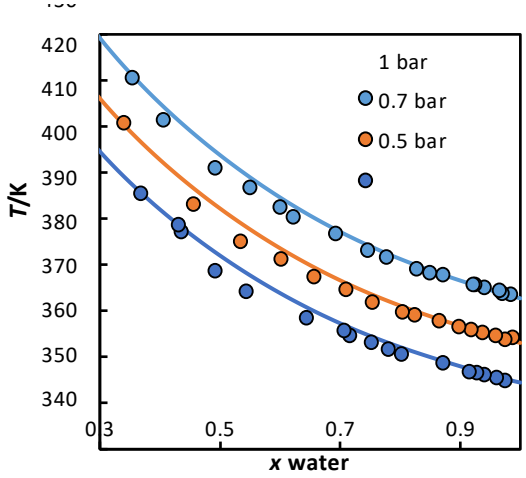

Figure S1 – VLE for water + triethylene glycol. Experimental data from Chouireb et al. [11]

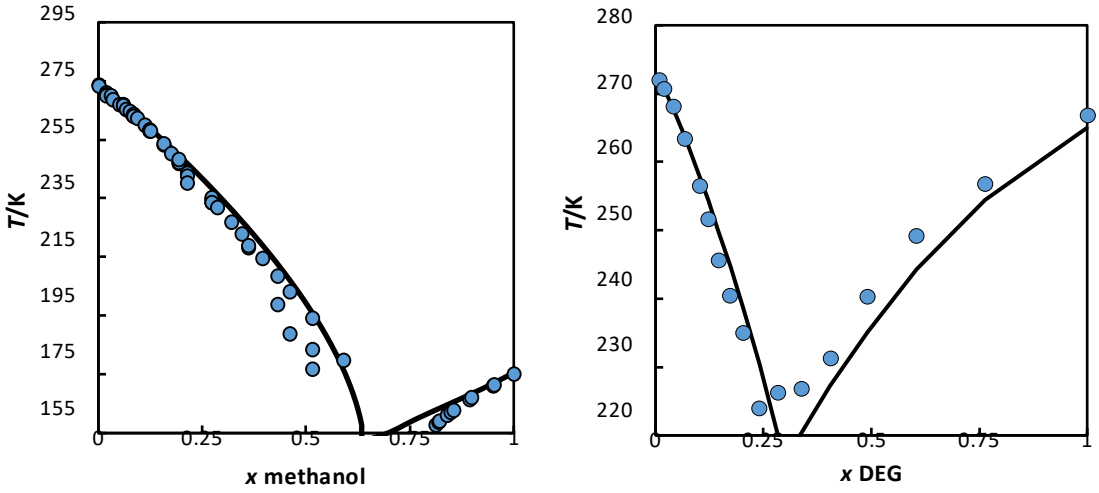

Figure S2 – SLE for water + methanol (left) and water + DEG (right). Experimental data from Chouireb et al. [11] and TRC. [12]

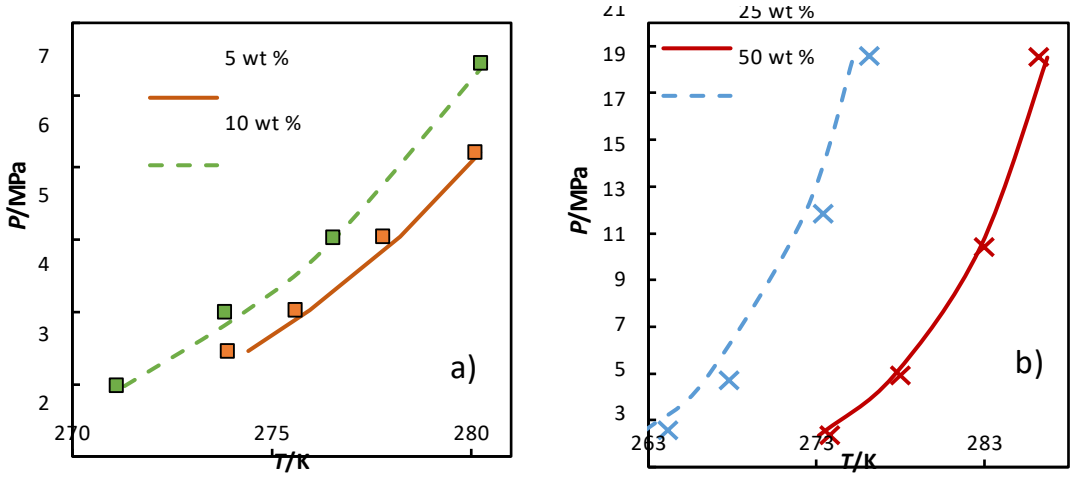

Figure S3 – Hydrate dissociation curves for mixtures of methane + water + inhibitor/guest hydrate former; Inhibitor/guest hydrate former a) ethanol, b) glycerol. wt % refers to weight percentage of inhibitor in aqueous solution. □ – Sloan and Koh [13]; x – Ng and Robinson [14]; + – Youn et al. [15].

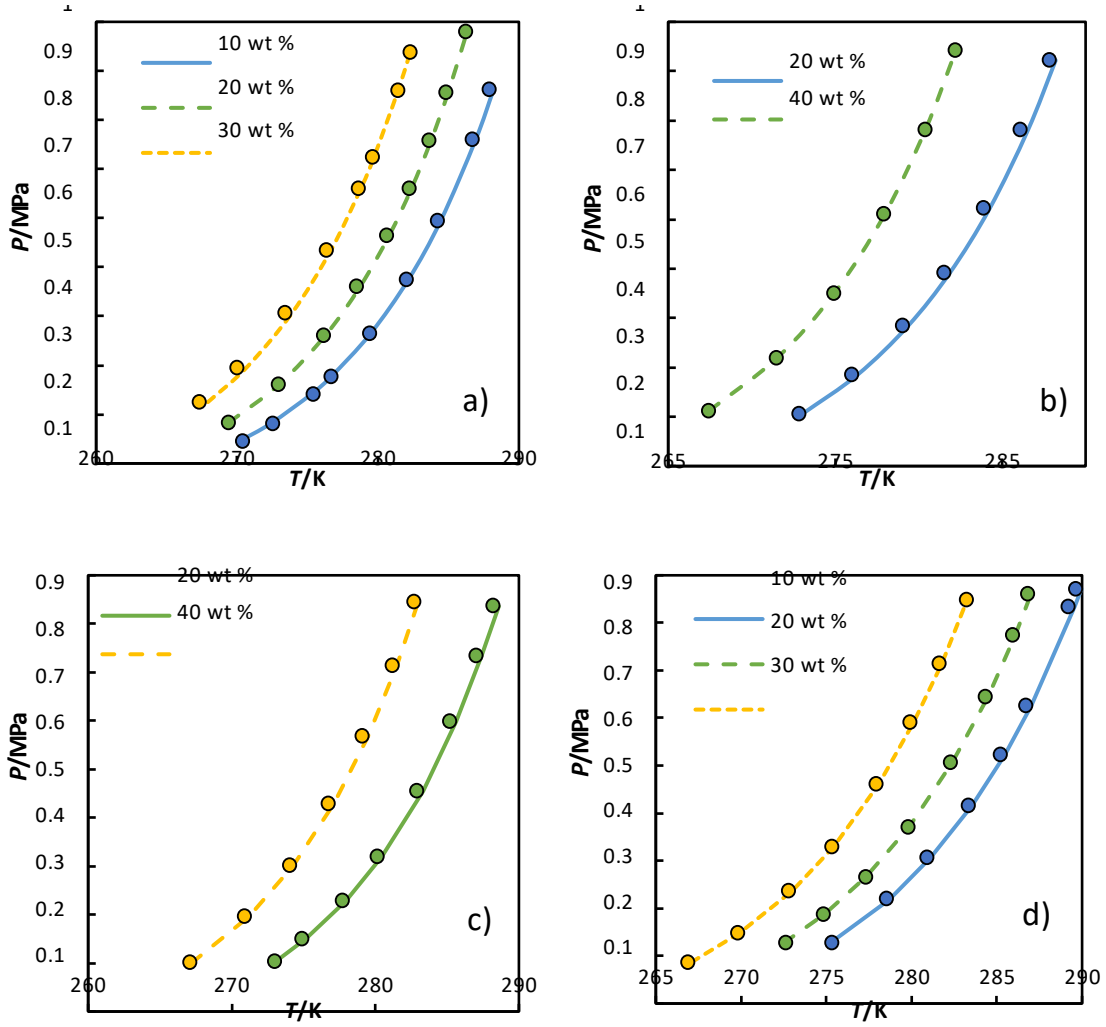

Figure S4 – Hydrate dissociation curves for mixtures of xenon + water + inhibitor; Inhibitor a) ethanol, b) glycerol, c) DEG, d) MEG. wt % refers to weight percentage of inhibitor in the aqueous phase. Single Lines – first sets; Double lines – second sets. ○ – Maekawa. [16]

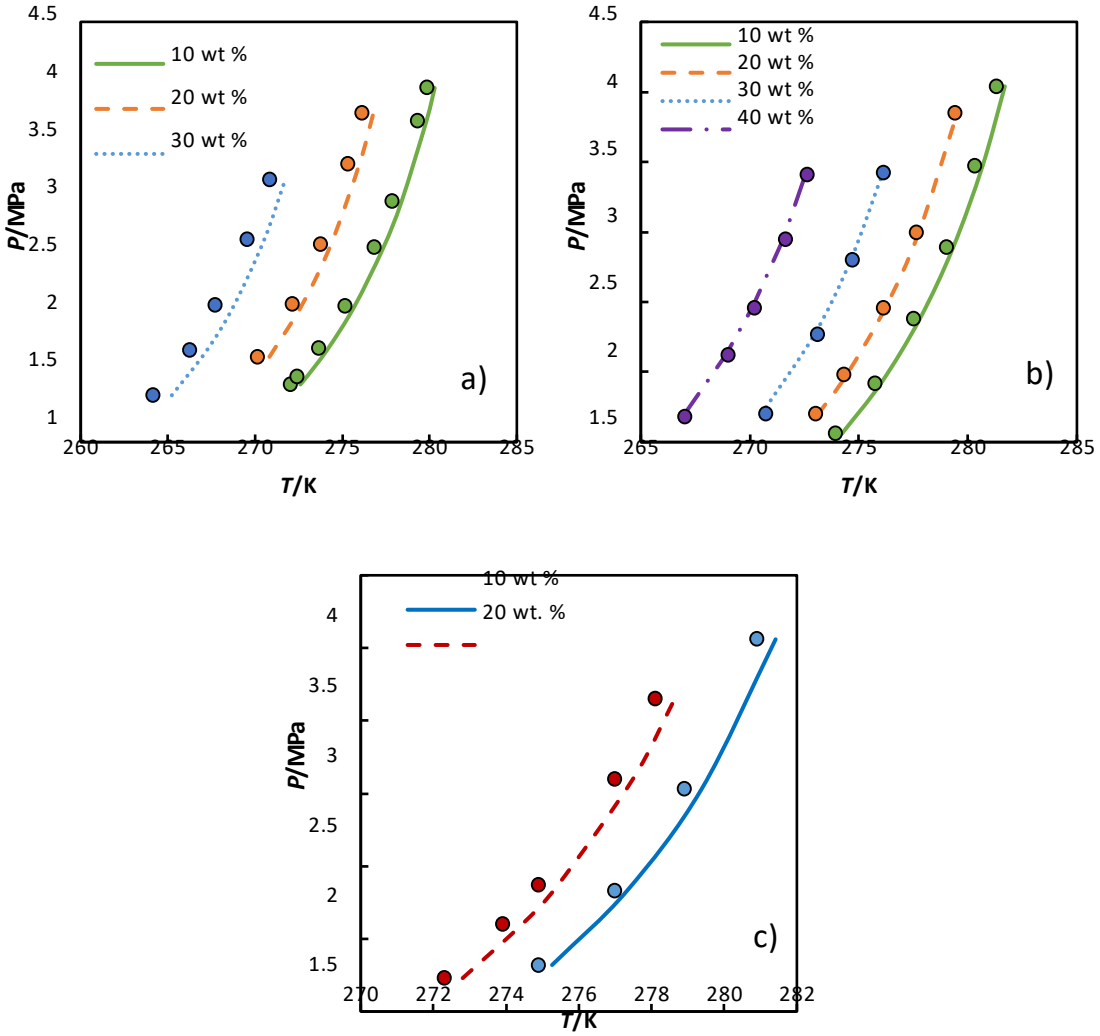

Figure S5 – Hydrate dissociation curves for mixtures of CO_2 + water + inhibitor; Inhibitor a) MEG, b) TEG c) DEG. wt % refers to weight percentage of inhibitor in aqueous solution. ○ – Maekawa. [17]

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