Corrigendum to “Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions” [Fluid Phase Equilibria, vol. 471, 2018, 74–87]

Wang, Tianyuan; Guittard, Philippe; Coquelet, Christophe; El Ahmar, Elise; Baudouin, Olivier; Kontogeorgis, Georgios M.

Published in:
Fluid Phase Equilibria

Link to article, DOI:
10.1016/j.fluid.2018.12.010

Publication date:
2019

Document Version
Peer reviewed version

Corrigendum to "Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions" [Fluid Phase Equilibria, Vol. 471, 2018, 74-87]

Tianyuan Wang[1,2], , Philippe Guittard[3], Christophe Coquelet[1] Elise El Ahmar[1], Olivier Bauduoin[3] and Georgios M. Kontogeorgis[2]

1: Mines ParisTech-PSL University Centre of Thermodynamics of Processes CTP, 35 rue Saint-Honore, 77305, Fontainebleau, France
2: Center for Energy Resources Engineering (CERE), Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
3: ProSim SA Immeuble Stratège A, 51 rue Ampère 31670, Labège, France

After careful comparison with the results of implanted PR-CPA EoS in Prosim software with the presented data in the paper, the authors found that some parameters in the table "PR-CPA EoS parameters for compounds for association compounds considered in this work "and the table "BIP values and ARD of total pressure between PR-CPA EoS results and experimental data for acid gas -alkanolamine binary system" were misprinted. The average absolute deviations and results presented in the paper are not influenced by this misprint.

Moreover, these parameters were also adjusted by PROSIM using their algorithms. The correct and new parameter values are presented in Tables 1 and 2 respectively. Figure 1 shows a comparison between the calculations using the two set of parameters. We can easily observe that with new parameters, the prediction is improved.

Table 1. PR-CPA EoS parameters for compounds for association compounds considered in this work.

Compound	scheme	a_0 /bar L^2 mol^{-2}($\times 10^{-1}$)	b /L mol^{-1}($\times 10^{2}$)	c_1	ε^{AiBj} /bar.L.mol^{-1}	β^{AiBj}	Tc /K	Range of Tr		ARD%[a]	
								For P_{sat}	For ρ_L	P_{sat}	ρ_L
MEA	4C	1.333	5.467	0.763	168.23	0.0142	671	0.42-0.92	0.43-0.61	1.8	0.6
MDEA	4C	3.339	11.346	0.695	201.76	0.0083	742	0.39-0.9	0.38-0.63	0.9	2
water	4C	0.123	1.445	0.674	170.48	0.0698	647	0.43-0.95	0.43-0.95	1	1.6
CO_2		0.397	2.661	0.701			304				
H_2S		0.492	2.696	0.517			373				

[a] ARD% = $1/np \times \Sigma|1 - \chi_i^{calc}/\chi_i^{exp}| \times 100\%$. χ: P_{sat} or ρ_L

Table 2 BIP values and ARD of total pressure between PR-CPA EoS results and experimental data for acid gas -alkanolamine binary system.

Binary	*T /K*	ARD_{Pt}%	k_{ij}[a]			β^{AiBj}	ε^{AiBj} /bar.L.mol^{-1}	$\beta^{AiBj'}$	$\varepsilon^{AiBj'}$ /bar.L.mol^{-1}	
			a	b×10^3 /K^{-1}	c×10^6 /K^{-2}					Source of BIP
CO_2-MEA	298-393	12	-6.99	29.9	-23.73	0.00411	408.62	0.00102	361.17	[1]
CO_2-MEA	298-393	12	-6.68816	30.7772	-23.2	0.00353698	441.451	0.00114328	351.619	PROSIM
CO_2-MDEA	313-413	11	6.53	-40.0	69.3	0.00487	345.69	NA	NA	[1]
H_2S-MEA	298-413	30*	-6.426	38.15	-49.94	0.00380	411.51	0.0170	178.26	[1]
H_2S-MDEA	311-388	13	0.8489	-2.834	8.461	0.01846	316.42	NA	NA	[1]

a: $kij = a + b \cdot T + c \cdot T^2$, ARD_{Pt} ARD on total pressure of acid gas-water-alkanolamine ternary systems, BIP: Binary Interaction Parameter

*: ARD% on partial pressure of H

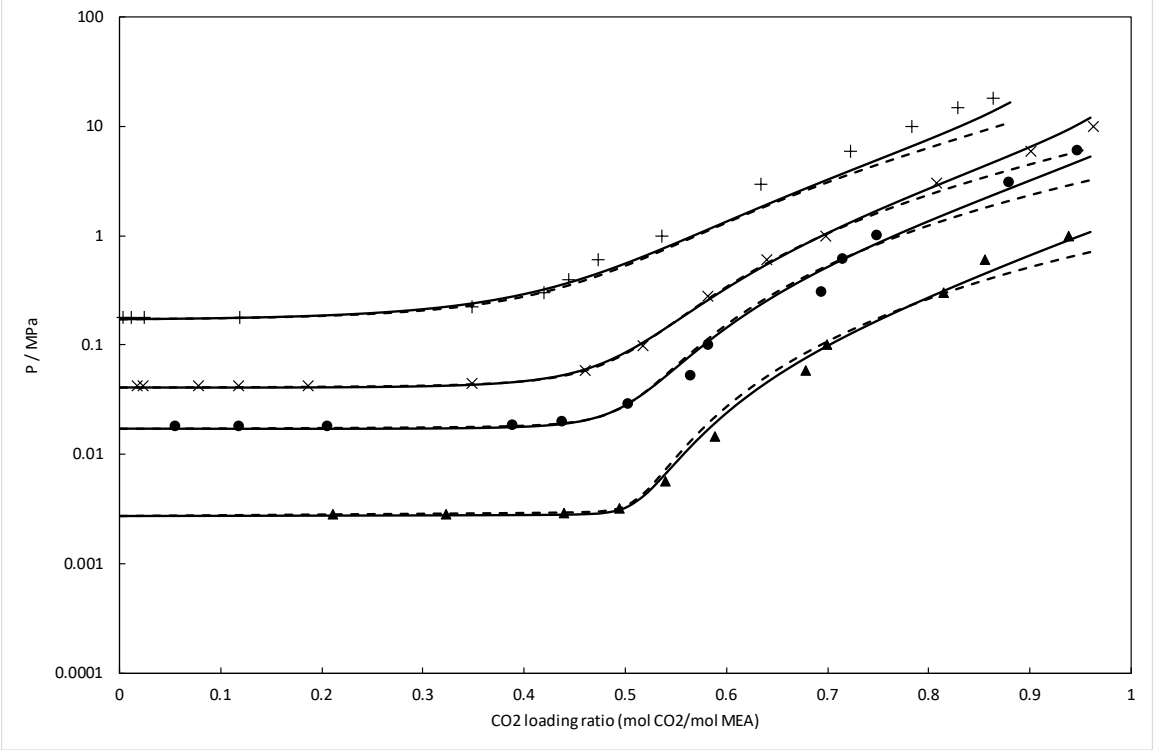

Figure 1: CO_2 solubility into H_2O-MEA mixture (30wt %): comparison of results using the two sets of parameters. Symbols: experimental data from Jou et al. [2]**. (▲)=298 K, (●)=333 K， (×)=353 K, (+)=393 K**

References

[1] T. Wang, E. El Ahmar, C. Coquelet, G. M. Kontogeorgis, Improvement of the PR-CPA equation of state for modelling of acid gases solubilities in aqueous alkanolamine solutions, 2018, Fluid Phase Equilibria, 471, 74-87.

[2] F.-Y. Jou, A.E. Mather, F.D. Otto, The solubility of CO_2 in a 30 mass percent monoethanolamine solution, Can. J. Chem. Eng. 73 (1995) 140–147.