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Addition/Correction

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Correction to "Analysis of Parameter Values in the van der Waals and Platteeuw Theory for Methane Hydrates Using Monte Carlo Molecular Simulations"

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In the original paper,[1] errors were made in the computation of the Langmuir constant using Monte Carlo integration when long-range methane−water and methane−methane interactions were included. We have repeated the calculations with the necessary corrections. These corrections affect Figures 4− 7, 10, and 11, as well as Tables 1−3. Here, we report the corrected figures and tables. In addition, the values of the residual Gibbs free energy ($g^{\beta}_{R_{w,0}}$) in Tables 1−3 are incorrect. These are also corrected in this manuscript. These corrections do not affect the major observations and conclusions presented in the original manuscript.

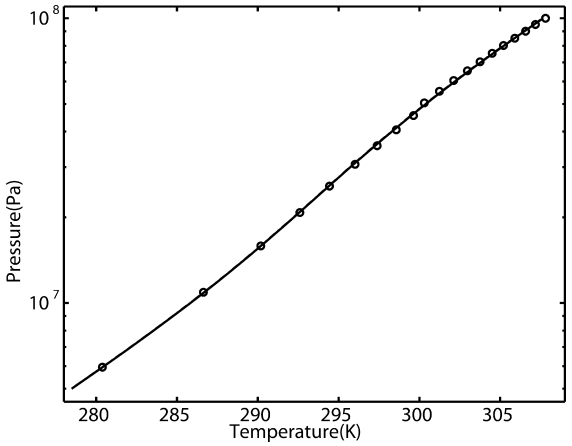

Figure 4. Pressure−temperature diagram showing the three-phase equilibrium between the vapor, liquid and hydrate phase using the TIP4P/Ice model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1_MC, vdWP-2_MC, and vdWP-3_MC are represented by the dotted−dashed line, the dashed line, and the full line, respectively.

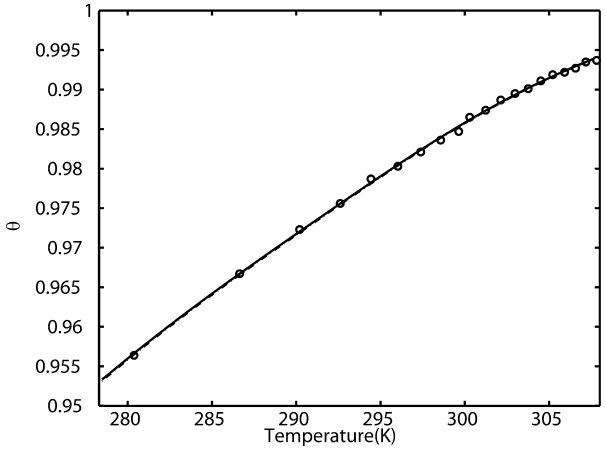

Figure 5. Occupancy versus temperature plot along the three-phase equilibrium between the vapor, liquid, and hydrate phase using the TIP4P/Ice model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1_MC, vdWP-2_MC, and vdWP-3_MC are represented by the dotted−dashed line, the dashed line, and the full line, respectively.

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Table 1. Optimized Parameter Values of the vdWP Theory Regressed from the Three-Phase Equilibrium Data Obtained from Simulations of Methane Hydrate Using the TIP4P/Ice Model[a]

	ε_{mw}/k_B (K)	σ_{mw} (Å)	$g^{\beta}_{R_{w,0}}$ (J/mol)	$h^{\beta}_{R_{w,0}}$ (J/mol)	$v^{\beta}_{w,0}$ (m^3/mol)
simulation	125.31	3.45	-2.77×10^4	-6.28×10^4	2.25×10^{-5}
vdWP-1	160.10	3.57	-2.75×10^4	-6.25×10^4	2.28×10^{-5}
vdWP-2	137.57	3.61	-2.75×10^4	-6.25×10^4	2.28×10^{-5}
vdWP-3	133.14	3.65	-2.73×10^4	-6.25×10^4	2.27×10^{-5}
vdWP-1_MC	160.72	3.58	-2.74×10^4	-6.25×10^4	2.28×10^{-5}
vdWP-2_MC	132.81	3.62	-2.74×10^4	-6.25×10^4	2.28×10^{-5}
vdWP-3_MC	129.59	3.66	-2.73×10^4	-6.24×10^4	2.27×10^{-5}

[a]The Gibbs free energy and the enthalpy are represented in terms of residual properties. Also listed are the interaction parameters used in the simulations and empty hydrate properties directly calculated from simulations.

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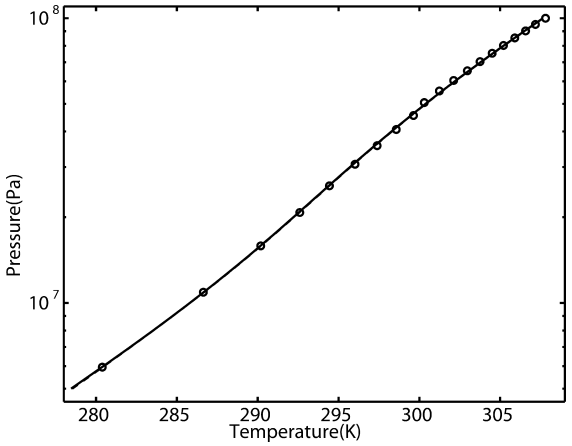

Figure 6. Pressure−temperature diagram showing the three-phase equilibrium between the vapor, liquid, and hydrate phase, using the TIP4P/Ice model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1 and vdWP-3_MC are represented by the dotted−dashed line and the full line, respectively. The methane−water interactions were kept equal to those used in simulations. The properties of the empty hydrates were obtained after regression with the simulation data.

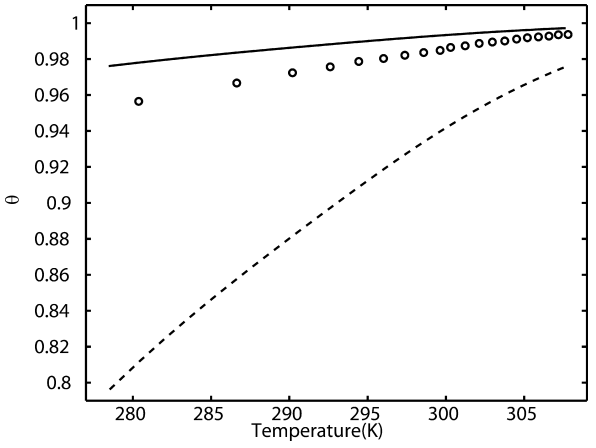

Figure 7. Occupancy versus temperature plot along the three-phase equilibrium between the vapor, liquid, and hydrate phase using the TIP4P/Ice model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1 and vdWP-3_MC are represented by the dotted−dashed line and the full line, respectively. The methane−water interactions were kept equal to those used in simulations.

Table 2. Optimized Empty Hydrate Parameter Values of the vdWP Theory Regressed from the Three-Phase Equilibrium Data Obtained from Simulations of Methane Hydrate Using the TIP4P/Ice Model[a]

	$g^{\beta}_{R_{w,0}}$ (J/mol)	$h^{\beta}_{R_{w,0}}$ (J/mol)	$v^{\beta}_{w,0}$ (m^3/mol)
simulation	-2.77×10^4	-6.28×10^4	2.25×10^{-5}
vdWP-1	-2.82×10^4	-6.29×10^4	2.30×10^{-5}
vdWP-3_MC	-2.74×10^4	-6.30×10^4	2.27×10^{-5}

[a]The Gibbs free energy and the enthalpy are represented in terms of residual properties. The methane−water and methane−methane interactions were kept equal to those used in the simulations. Also, listed are the empty hydrate properties directly calculated from simulations.

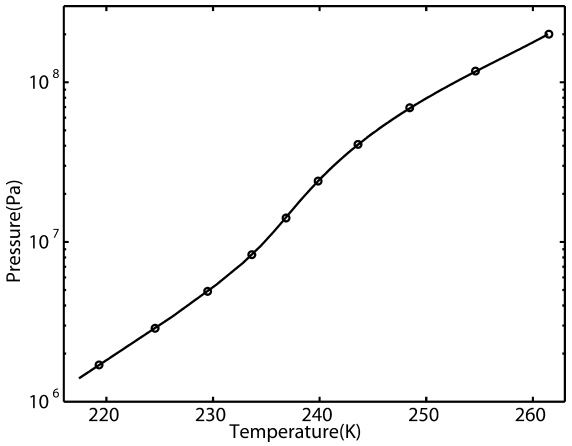

Figure 10. Pressure−temperature diagram showing the three-phase equilibrium between the vapor, liquid, and hydrate phase using the SPC/E model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1_MC, vdWP-2_MC, and vdWP-3_MC are represented by the dotted−dashed line, the dashed line, and the full line, respectively.

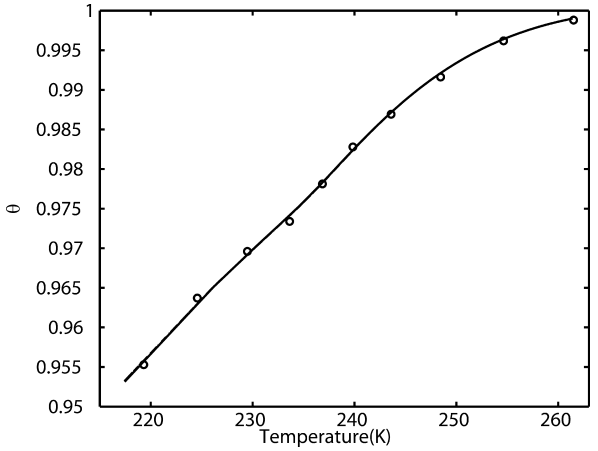

Figure 11. Occupancy versus temperature plot along the three-phase equilibrium between the vapor, liquid, and hydrate phase using the SPC/E model for water. The circles represent equilibrium points calculated from simulations. The predictions from vdWP-1_MC, vdWP-2_MC and vdWP-3_MC are represented by the dotted−dashed line, the dashed line, and the full line, respectively.

REFERENCES

(1) Ravipati, S.; Punnathanam, S. N. Analysis of Parameter Values in the van der Waals and Platteeuw Theory for Methane Hydrates Using Monte Carlo Molecular Simulations. *Ind. Eng. Chem. Res.* **2012**, *51*, 9419−9426.

Table 3. Optimized Parameter Values of the vdWP Theory Regressed from the Three-Phase Equilibrium Data Obtained from Simulations of Methane Hydrate Using the SPC/E Model[a]

	ε_{mw}/k_B (K)	σ_{mw} (Å)	$g^{\beta}_{R_{w,0}}$ (J/mol)	$h^{\beta}_{R_{w,0}}$ (J/mol)	$v^{\beta}_{w,0}$ (m^3/mol)
simulation	107.44	3.45	-2.58×10^4	-5.57×10^4	2.16×10^{-5}
vdWP-1	148.72	3.58	-2.54×10^4	-5.53×10^4	2.17×10^{-5}
vdWP-2	127.97	3.62	-2.54×10^4	-5.53×10^4	2.17×10^{-5}
vdWP-3	130.75	3.67	-2.50×10^4	-5.50×10^4	2.16×10^{-5}
vdWP-1_MC	152.09	3.59	-2.53×10^4	-5.53×10^4	2.17×10^{-5}
vdWP-2_MC	126.65	3.63	-2.52×10^4	-5.52×10^4	2.17×10^{-5}
vdWP-3_MC	131.32	3.69	-2.48×10^4	-5.48×10^4	2.16×10^{-5}

[a]The Gibbs free energy and the enthalpy are represented in terms of residual properties. Also listed are the interaction parameters used in the simulations and empty hydrate properties directly calculated from simulations.

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