

ERRATA

Erratum: "Computer simulations of vapor–liquid phase equilibria of *n*-alkanes" [J. Chem. Phys. 102, 2126 (1995)]

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We have recently found an error in our Gibbs-ensemble Monte Carlo computer program which had been used to calculate the vapor–liquid coexistence curves reported in the original paper.¹ This error was caused by a missing factor of σ^3 in the analytical tail corrections used to estimate the interactions beyond a spherical potential truncation.

The results reported in Ref. 1 for the OPLS and de Pablo models are not affected by this error, because a spherical truncation at 11.5 Å without tail corrections was used for the OPLS model and the minimum image convention was employed for the de Pablo model. However, the numerical results reported for the Toxvaerd model and the new model proposed in Ref. 1 are in error. The values of the Lennard-Jones parameter σ are 3.527 Å (Toxvaerd model) and 3.93 Å (new model). Thus, in the former case the tail corrections were underestimated by a factor of 44 and in the latter by 61. These large factors mean that the results reported in Ref. 1 correspond in practice to calculations performed without tail corrections.

TABLE I. Critical properties obtained from the simulations (using a critical exponent $\beta=0.32$). Subscripts show the statistical uncertainty of the final digit. See Table III of Ref. 1.

	T_c [K]	ρ_c [g/ml]	p_c [MPa]
<i>n</i> -pentane			
Original (Ref. 1)	494 ₄	0.223 ₅	3.9 ₅
Corrected	510 ₄	0.224 ₆	3.8 ₇
Experiment	470	0.230	3.4
<i>n</i> -octane			
Original (Ref. 1)	577 ₃	0.229 ₅	2.7 ₅
Corrected	610 ₅	0.222 ₉	2.5 ₉
Experiment	569	0.232	2.5
<i>n</i> -dodecane			
Original (Ref. 1)	659 ₇	0.223 ₇	2.3 ₅
Corrected	703 ₇	0.227 ₆	2.4 ₆
Experiment	658	0.226	1.8

We have repeated the calculations for *n*-pentane, *n*-octane, and *n*-dodecane for the new model using proper values for the tail corrections. The corrected critical points and coexistence densities are reported in Tables I and II. The critical temperatures are shifted to higher values (by 4 to 6%), but the critical densities and pressures are affected to a lesser extent. The coexistence curves for the Toxvaerd model should shift in a similar way to higher temperatures, i.e., improving the agreement with the experimental data. The qualitative results, such as the chain-length dependencies of the critical properties, are not affected by the error.

TABLE II. Saturated vapor and liquid densities. Subscripts show the statistical uncertainty of the final digit. See Table VI of Ref. 1.

T [K]	ρ_{vap} [g/ml]		ρ_{liq} [g/ml]	
	Ref. 1	Corrected	Ref. 1	Corrected
<i>n</i> -pentane				
375	0.014 ₅	0.010 ₁	0.528 ₅	0.548 ₂
400	0.021 ₁₅	0.017 ₂	0.500 ₁₀	0.516 ₄
425	0.030 ₁₀	0.027 ₂	0.475 ₁₀	0.484 ₃
445	0.047 ₁₀	0.042 ₁	0.430 ₁₀	0.468 ₉
475	0.090 ₁₀	0.066 ₁	0.380 ₁₀	0.416 ₈
<i>n</i> -octane				
435	0.008 ₅	0.006 ₁	0.573 ₇	0.589 ₃
485	0.028 ₃	0.016 ₃	0.521 ₄	0.540 ₅
510	0.033 ₃	0.021 ₃	0.468 ₅	0.510 ₇
550	0.08 ₁	0.037 ₃	0.40 ₁	0.460 ₈
575	N/A	0.063 ₃	N/A	0.40 ₂
<i>n</i> -dodecane				
450	0.005 ₅	0.0012 ₂	0.625 ₅	0.637 ₂
500	0.012 ₅	0.004 ₁	0.576 ₅	0.594 ₇
550	0.014 ₅	0.012 ₁	0.518 ₅	0.558 ₃
600	0.060 ₁₀	0.026 ₄	0.437 ₂₀	0.498 ₅
615	0.055 ₁₀	0.031 ₅	0.45 ₁	0.478 ₇

¹B. Smit, S. Karaborni, and J. I. Siepmann, J. Chem. Phys. **102**, 2126 (1995).