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**Corrigendum to “Vapor-liquid equilibrium and molecular simulation data
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(R-1234ze(E)) mixture at temperatures from 283.32 to 353.02 K and
pressures up to 7.6 MPa” [International Journal of Refrigeration, Volume
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Rémi Fauve², Christophe Coquelet^{2*}, Céline Houriez², Pierre-Arnaud Artola^{3a}, Elise El Ahmar², Bernard Rousseau^{3b}

1 Institute of Refrigeration and Cryogenics, Shanghai Jiao Tong Univ, 800 Dongchuan Rd, 200240 Shanghai, China

2 Mines ParisTech, PSL Research University, CTP – Centre of Thermodynamics of Processes 35, rue Saint Honoré 77305 Fontainebleau Cedex France

3a: Laboratoire de Chimie Physique, Université Paris-Sud bâtiment 349, 310 Rue Michel Magat, 91405 Orsay, France

3b: Laboratoire de Chimie Physique, Université Paris-Sud bâtiment 349, UMR 8000 CNRS, 310 Rue Michel Magat, 91405 Orsay, France

*: Corresponding author: christophe.coquelet@mines-paristech.fr (tel: +33164694962 Fax: +33164694968).

After careful analysis of the GEMC results for phase composition presented in the paper, we noticed that the data at 353.02 K and 5.623 MPa seemed out of trend when compared to the data of the same system at other conditions. Our hint was reinforced by fitting power laws with asymptotic behavior at critical point [1] [2] [3] simultaneously on molecular simulation phase densities and compositions. The critical phase behavior data calculated by power laws with asymptotic behavior at critical point (Eq. (1)) are presented in Table 1 and plotted on Figures 1 and 2.

$$\begin{aligned}\frac{y+x}{2} - x_c &= \lambda_1(P_c - P) \\ y - x &= \lambda_2(P_c - P) + \mu(P_c - P)^\beta \\ \frac{\rho_v + \rho_l}{2} - \rho_c &= \lambda(P - P_c) \\ \rho_l - \rho_v &= \gamma(P - P_c)^\beta\end{aligned}\tag{1}$$

The molecular simulation was restarted with a slightly different global composition of the CO₂ (1) + R-1234ze(E) (2) mixture ($x_{\text{CO}_2} = 0.45$ instead of $x_{\text{CO}_2} = 0.42$). By monitoring properties such as pressure, density and composition of each simulation box, plotted in Figure 3, we can conclude that the

system with a global composition of $x_{\text{CO}_2} = 0.45$ has reached a thermodynamic equilibrium at around 50 million attempted Monte Carlo moves (MC steps). The corrected GEMC results for this system are shown in Table 2. This correction induces a slight modification of mean absolute deviations between GEMC simulation results and experimental data ($\Delta P = 0.074$ MPa, $\Delta x_1 = 0.023$ and $\Delta y_1 = 0.037$), but that doesn't influence the conclusion presented in the paper.

Comment

Phase compositions and densities, at a given pressure, temperature and global composition, can be extracted from a single GEMC simulation. Hence, the critical coordinates can be predicted, using power laws with asymptotic behavior at critical point, taking into account both phase compositions and densities. The static-analytic method used in this work to perform the isothermal VLE data measurement can only deliver phase compositions, and another method is required to get experimental phase densities.

Comparison of phase compositions predictions between GEMC simulations and REFPROP version 9.0 and 10.0 is already presented in the paper. The critical points predicted by power laws with asymptotic behavior at critical point fitted on GEMC results are plotted on Figures 1 and 2. On Figure 2, predicted phase densities are compared to calculated phase densities, provided by the Peng-Robinson equation of state (PR EoS), despite lack of experimental phase densities. The critical composition and density are both overestimated by GEMC and REFPROP predictions, but GEMC predictions are more accurate. Near critical point, GEMC and REFPROP version 10.0 predictions are both more accurate for the liquid phase rather than the vapor phase.

In conclusion, GEMC simulations, with molecular models only fitted with pure compound data, provide better vapor-liquid data predictions of the $\text{CO}_2 + \text{R-1234ze(E)}$ mixture near critical point than REFPROP version 10.0, which highly overestimates the critical composition, despite using binary interaction parameters fitted over Raabe's molecular simulation data [4] for the mixture $\text{CO}_2 + \text{R-1234ze(E)}$, at lower temperatures. Experimental phase densities for the $\text{CO}_2 (1) + \text{R-1234ze(E)}$ mixture are needed to do quantitative comparison with the presented predictions.

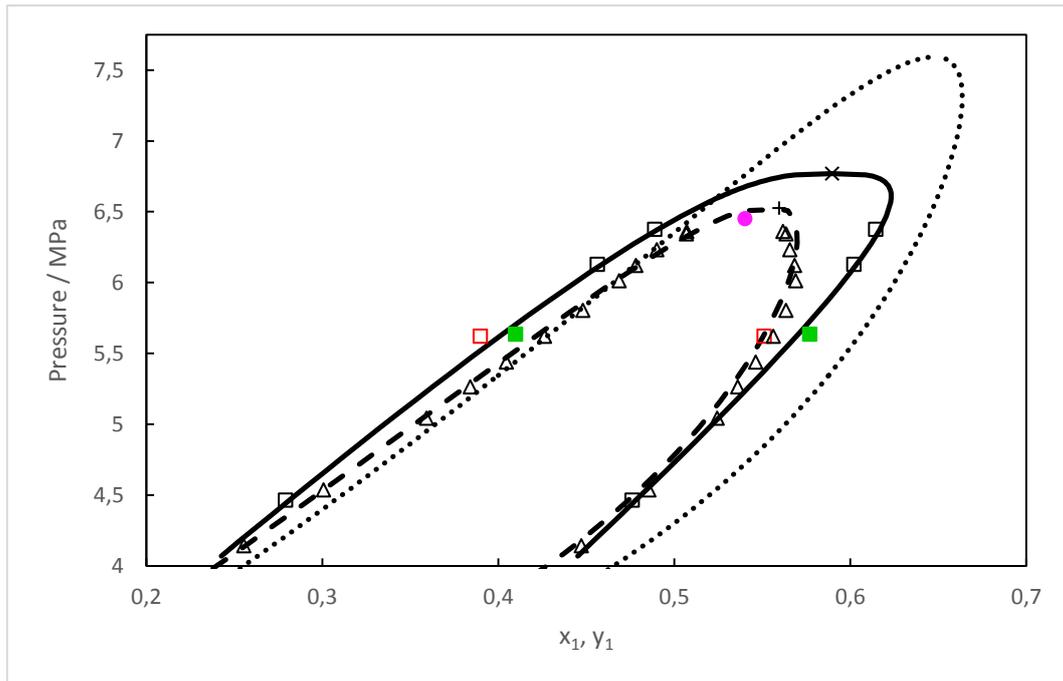


Figure 1: Pressure as a function of CO₂ mole fraction in the CO₂(1) + R-1234ze(E) (2) mixture at 353.02 K. □: GEMC simulations (◻: previous data, ◼: corrected data). Solid line: power laws with asymptotic behavior at critical point on GEMC results. ×: critical point predicted by power laws on GEMC results. Δ: experimental isothermal VLE data. ●: critical point predicted by power laws on experimental data. Dashed line: calculated with PR EoS, Wong-Sandler mixing rules and NRTL activity coefficient model. +: critical point calculated using our model. Dotted line: calculated using REFPROP 10.0 [5].

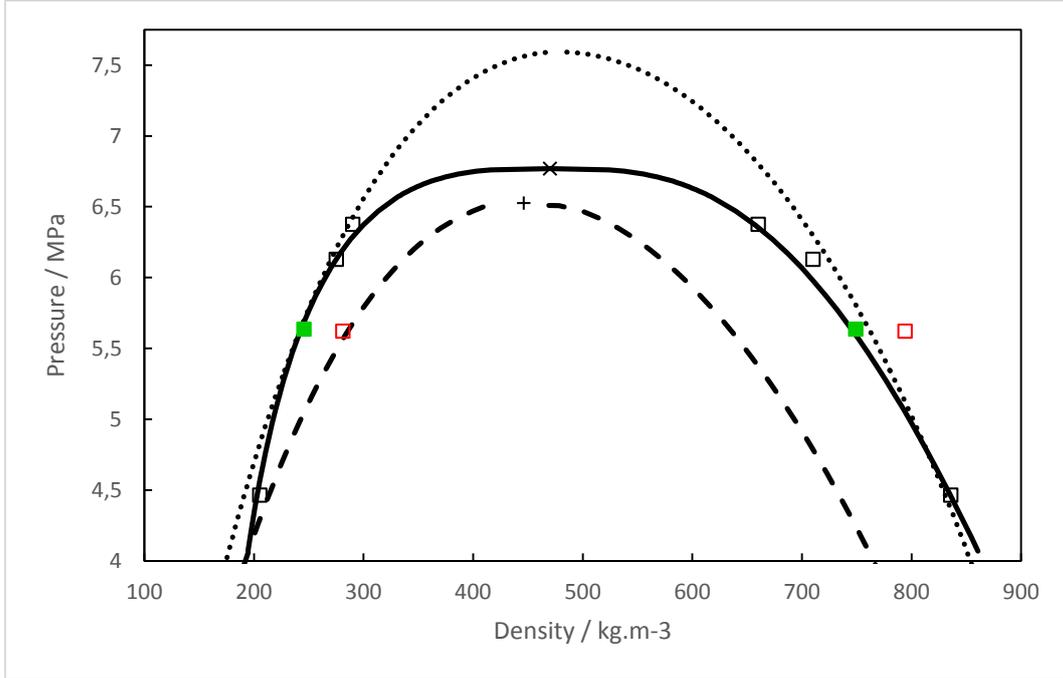


Figure 2: Pressure as a function of density in the CO₂ (1) + R-1234ze(E) (2) mixture at 353.02 K. □: GEMC simulations (□: previous data, ■: corrected data). Solid line: power laws with asymptotic behavior at critical point on GEMC results. ×: critical point predicted by power laws on GEMC results. Dashed line: calculated with PR EoS, Wong-Sandler mixing rules and NRTL activity coefficient model. +: critical point calculated using our model. Dotted line: calculated using REFPROP 10.0 [5].

Table 1: Predictions using power laws with asymptotic behavior at critical point of critical composition (x_{c1}), pressure (P_c) and density (ρ_c) of the CO₂ (1) + R-1234ze(E) (2) binary system at 353.02 K, with GEMC results.

	P_c	x_{c1}	ρ_c	λ	γ	λ_1	λ_2	μ
GEMC	6.770	0.5896	469.9	-21.29	482.1	-0.01688	-0.09103	0.1797

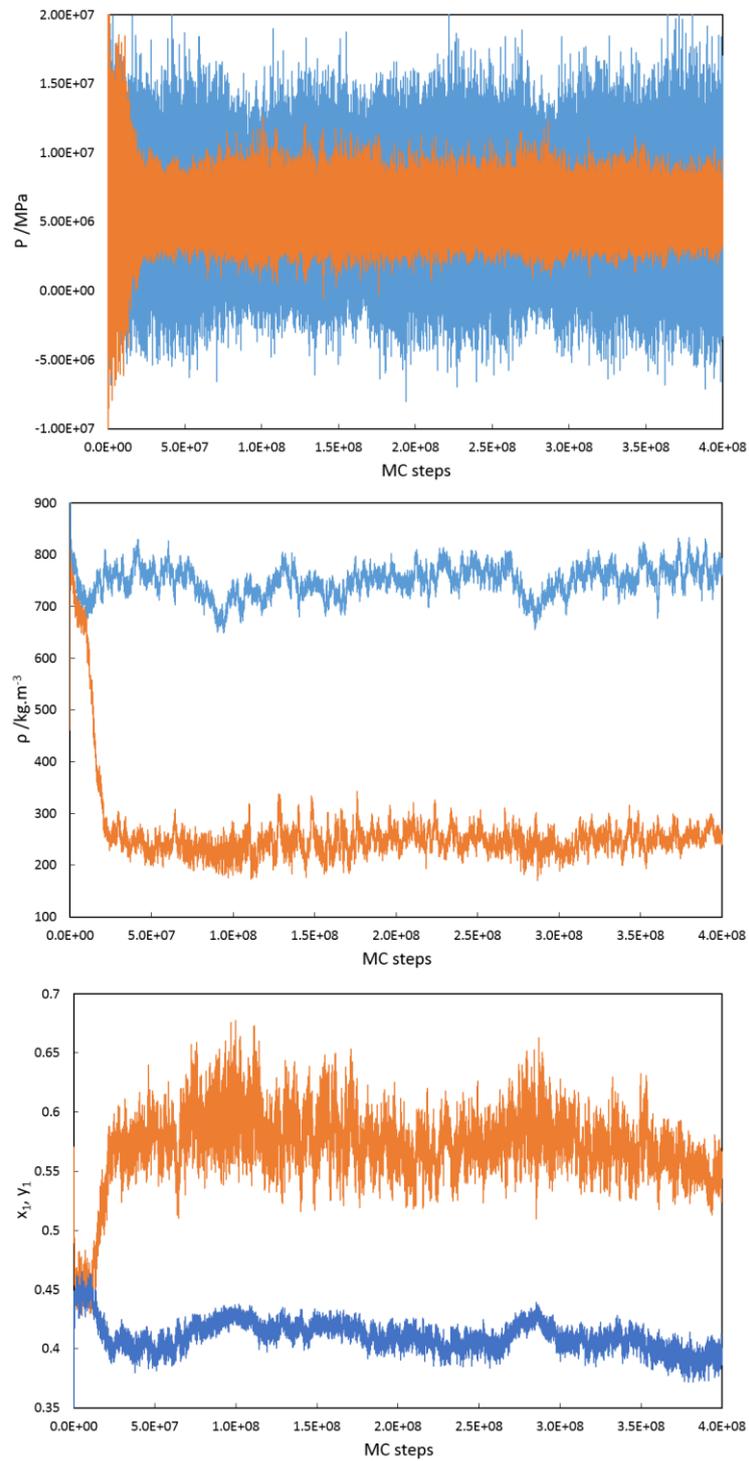


Figure 3: Evolution of pressures, densities and compositions of CO_2 in the CO_2 (1) + R-1234ze(E) (2) mixture at 353.02 K during GEMC simulations, with a global composition of $x_{\text{CO}_2} = 0.45$. Blue solid line: simulation box A. Orange solid line: simulation box B.

Table 2: GEMC simulation results for the Vapor Pressure P , Liquid-Phase Molar Fraction x , Gas-Phase Mole Fraction y , Saturated Liquid Density ρ^L and Saturated Vapor Density ρ^V of the VLE for the CO₂ (1) + R-1234ze(E) (2) mixture system^a

P /MPa	$u(P)$ /MPa	x_1	$u(x_1)$	y_1	$u(y_1)$	ρ^L /kg.m ⁻³	$u(\rho^L)$ /kg.m ⁻³	ρ^V /kg.m ⁻³	$u(\rho^V)$ /kg.m ⁻³
$T: 353.02\text{ K}$									
5.637	0.070	0.4097	0.0063	0.5769	0.0089	749	13	245.5	6.6

^a $u(P)$, $u(x_1)$, $u(y_1)$, $u(\rho^L)$ and $u(\rho^V)$ are the statistical uncertainties for a 99% confidence interval (i.e. $k = 2.5$)

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