

ADDITIONS AND CORRECTIONS

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Equation of State for Small, Large, Polydisperse, and Associating Molecules: Extension to Fluid Mixtures. Stanley H. Huang and Maciej Radosz*

Page 2002. Appendix: the same symbols as defined in the Nomenclature section are used. SAFT expressions for the compressibility factor and fugacity coefficient are added, and the expression for a^{res} is corrected.

Equation A24 should be

$$\frac{a^{\text{res}}}{RT} = \frac{3\frac{BC}{D} - \frac{C^3}{D^2}}{1 - \zeta} + \frac{\frac{C^3}{D^2}}{(1 - \zeta)^2} + \left[\frac{C^3}{D^2} - A \right] \ln(1 - \zeta) + F + E \sum_i \sum_j D_{ij} G^i \left[\frac{\zeta}{\tau} \right]^j + H \quad (\text{A24})$$

This correct form of eq A24 was actually used in calculations presented in the original paper.

Using the same symbols as in the Appendix, and following Topliss (1985), here is an expression for the compressibility factor Z :

$$Z = 1 + \rho \left[\frac{\partial \tilde{a}}{\partial \rho} \right]_{T, \mathbf{X}} = 1 + \rho \left[\left[\frac{\partial \tilde{a}}{\partial \rho} \right]_{T, \beta} + \sum_{i=1}^8 \left[\frac{\partial \tilde{a}}{\partial \beta_i} \right]_{T, \rho, \beta_{j \neq i}} \left[\frac{\partial \beta_i}{\partial \rho} \right]_{T, \mathbf{X}} \right] \quad (\text{A92})$$

where the boldface symbols represent vectors, and where

$$\tilde{a}(\rho, T, \mathbf{X}) = \tilde{a}[\rho, T, \beta(\rho, T, \mathbf{X})] = \frac{a^{\text{res}}}{RT} \quad (\text{A93})$$

An expression for the log fugacity coefficient $\ln \phi_i(\rho, T, \mathbf{X})$ is

$$\ln \phi_i = \left[\frac{\partial(N\tilde{a})}{\partial n_i} \right]_{\rho, T, n_{j \neq i}} + (Z - 1) - \ln Z \quad (\text{A94})$$

where N is the total number of moles and the residual is defined with respect to a mixture of ideal gases at the same ρ , T , and \mathbf{X} .

$$\left[\frac{\partial(N\tilde{a})}{\partial n_i} \right]_{\rho, T, n_{k \neq i}} = \tilde{a} + \left[\frac{\partial \tilde{a}}{\partial X_i} \right]_{\rho, T, X_{k \neq i}} - \sum_j X_j \left[\frac{\partial \tilde{a}}{\partial X_j} \right]_{\rho, T, X_{k \neq j}} \quad (\text{A95})$$

where

$$\left[\frac{\partial \tilde{a}}{\partial X_i} \right]_{\rho, T, X_{k \neq i}} = \sum_{l=1}^8 \frac{\partial \tilde{a}}{\partial \beta_l} \frac{\partial \beta_l}{\partial X_i} \quad (\text{A96})$$

and

$$\left[\frac{\partial \tilde{a}}{\partial X_j} \right]_{\rho, T, X_{k \neq j}} = \sum_{l=1}^8 \frac{\partial \tilde{a}}{\partial \beta_l} \frac{\partial \beta_l}{\partial X_j} \quad (\text{A97})$$

Ram Gupta of the University of Texas in Austin kindly drew our attention to the incorrect form of eq A24 in the original paper.