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## Comment on "A comparative study of numerical methods for calculating phase equilibria in fluid mixtures from an equation of state" by K. Fotouh and K. Shukla

(Received 21 August 1996)

The contribution of K. Fotouh and K. Shukla (1996, *Chem. Engng Sci.* **51**(15), 3763-3771) is misleading because it confuses the accuracy of an equation-of-state model with the precision and incorrect solutions of computational algorithms.

Once the model parameters are defined, the Redlich-Kwong-Soave equation of state (and other similar models) provides unique, unambiguous predictions of phase equilibrium and other thermodynamic properties. It is these unique solutions—and these unique solutions only—that should be used to evaluate the accuracy and range of validity of the model, by comparison with experimental data.

Industrial practitioners like me recognize the difficulty and the value of obtaining the precise and correct solution of EOS models, particularly in the critical region. In this context, the contribution of Fotouh and Shukla serves a valuable purpose. Computational algorithms can and should be compared for their computational efficiency and their ability to converge to the correct solution within a defined

tolerance. But experimental data have no role in this comparison, other than approximately identifying relevant regions for the comparison. It is meaningless and misleading to compare varying results of several computational algorithms to experimental data. There is only one model result—the correct one—that should be compared to experimental data.

Similar to experimental measurements, modeling suffers from accuracy and precision problems. An important value of modeling is that good practice (i.e. good computational techniques) will largely eliminate the precision problems. In any case, the distinction between accuracy and precision must be retained.

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