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Short communication

Improved solution windows for the resolution of the Rachford-Rice equation

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Abstract

In a recent study (D.V. Nichita, C.F. Leibovici, A Rapid and Robust Method for Solving the Rachford-Rice Equation Using Convex Transformations, Fluid Phase Equilib. 353, 2013, 38-49) we have shown that using appropriate changes of variables the original function can be transformed in convex functions for which the sufficient condition of monotonic convergence of the Newton method is fulfilled, thus Newton iterations can be used without interval control. For the proposed algorithms, the quality of the initial guess, thus the convergence speed, are directly related to the existence of narrow solution windows. In this work, new, extremely simple solution windows are proposed, which depends only on feed compositions. It is proved that novel solution windows are always smaller than previously proposed ones. Numerical experiments are carried out for a very large number of randomly generated flashes, showing that the use of new solution windows systematically decreases the number of iterations required for convergence. In the range of number of components usually encountered in compositional reservoir simulations, the reduction in number of iterations is about 15 % as compared to the fastest previous formulation.

Keywords: Rachford-Rice equation, flash calculations, convex function, monotonic convergence, Newton methods, solution window

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