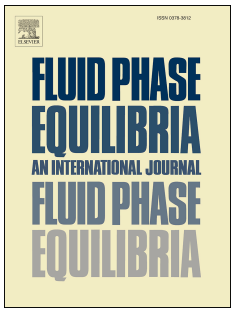

Chemical and phase equilibrium calculations by Gibbs energy minimization using deterministic methods based on globally convergent branch and bound algorithms

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Chemical and phase equilibrium calculations by Gibbs energy minimization using deterministic methods based on globally convergent branch and bound algorithms

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Abstract

In this paper, a modified version of the well-known branch-and-bound algorithm, αBB, as well as an underestimator-independent branch-and-bound method have been applied to determine the chemical and phase equilibrium conditions of isothermal and isobaric systems by means of Gibbs energy minimization. The original αBB algorithm mathematically guarantees global convergence by successively generating convex underestimators and solving convex subproblems. These underestimators, however, are in general not tight and ultimately may lead to very large numbers of iterations. The branch-and-bound algorithms presented, despite not guaranteeing global convergence, have proven to be effective for solving Gibbs energy minimization problems without prohibitive dependences on the thermodynamic models employed, requirements of problem-specific parameter tuning, or the need for significant computational effort. Eight benchmark chemical and phase equilibria

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