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An enhanced branch and bound algorithm for phase stability testing of multicomponent mixtures

Tuesday, 31 May 2022 10:45 (15 minutes)

The stability of matter is one of the fundamental problems of physics. In this contribution, we examine phase stability. From the mathematical point of view, the problem of coexistence or separation of phases can be formulated as a global optimization problem. We consider VTN-stability testing, i.e. the phase compostion of a mixture under fixed concentrations and temperature. Our goal is to predict whether the phase composition of a mixture is stable or unstable. In other words, if the mixture stays in a single phase or splitting into multiple phases occurs. Mikyška and Firoozabadi (Mikyška, J.; Firoozabadi A. 2012) derived a criterion for the VTN-phase stability which leads to solving an optimization problem. Mikyška and Smejkal (Smejkal T.; Mikyška J. 2020) proposed to solve this problem with the branch and bound algorithm with the use of a convex concave split. In this contribution, we are going to improve the algorithm with more effective bounding strategy. This improvement is achieved using the necessary condition of optimality. In the bounding step of the algorithm, before solving an underestimated convex optimization, we check whether the pressure (given by the Peng-Robinson equation of state) is feasible. If it is not the case, we can exclude the corresponding part of the feasible set from the search. The Peng-Robinson equation of state is not convex and therefore leads to a non convex optimization which is computationally expensive. We propose to use a less precise estimate of the global minimum of the pressure. This estimate can be found by comparing the finite number of the values of the tangent plane to a concave overestimate of the Peng-Robinson equation of state. Another benefit of this additional step is to avoid the optimization of an underestimated objective function. Suggested method is tested on several concrete examples.

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Time Block Preference

Time Block B (14:00-17:00 CET)

Participation

In person

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