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Robust and efficient Trust-Region based stability analysis and multiphase flash calculations

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ABSTRACT

Multiphase flash calculations and phase stability analysis are central in compositional reservoir and chemical process simulators. For instance, in some simulations, a huge amount of phase equilibrium calculations is required (the most important part of the computational effort). Moreover, a single failure may cause significant error propagations leading to false solutions. Thus, it is imperative that calculation algorithms are efficient and highly robust. The most difficult regions in mixture phase envelopes are in the vicinity of singularities: critical points for flash calculations and the stability test limit locus for stability analysis. For these conditions, all algorithms have difficulties to converge. Traditionally, a number of successive substitution iterations (SSI) are performed before switching to the second-order Newton method (many SSI iteration may be required before switch very close to singularities). The Trust-Region method has the advantage of performing a Newton step whenever the Hessian is definite positive; otherwise, the Trust-Region corrects the Hessian matrix by adding a diagonal element to make it positive definite, thus a descent direction is guaranteed. The Trust-Region limits the solution within a trust-radius, which is updated automatically at each iteration level, depending on the quality of the quadratic approximation. If the function is convex, the trust-radius enables larger changes in iteration variables, otherwise restricted steps are used to ensure a progress towards the solution. The proposed Trust-Region algorithm, as well as a hybrid methodology that combines SSI, Newton and Trust-Region steps, are tested for multiphase flash calculations and stability analysis on a variety of mixtures involving hydrocarbon components, carbon dioxide and hydrogen sulfide, exhibiting complicated phase envelopes. The proposed method compares favorably to the widely used SSI-Newton methods with various independent variables. The more difficult a test point is, the more spectacular the algorithm acts from both efficiency and reliability perspectives.

1. Introduction

Multiphase flash calculations and stability analysis testing are in the center of compositional reservoir and chemical process simulators. For instance, in compositional hydrocarbon reservoir simulation, a huge amount of phase equilibrium calculations is required (the most important part of the computational effort): in each reservoir grid block, at each time step and at each iteration level. Moreover, a single failure may cause significant error propagations leading to false solutions. Thus, it is imperative that calculation algorithms are efficient and highly robust: reliability has to be kept ensuring in the same time a reasonably fast convergence even in very difficult cases.

The resolution of the multiphase flash problem requires the minimization of the Gibbs free energy [1] and of the tangent-plane distance (TPD) function [2] for phase stability testing. Traditionally, first-order successive substitution (SSI) iterations are performed before switching to the second-order Newton method. In most of the cases, the Newton method works fine (convergence to the solution is achieved in a few iterations) provided the Hessian is positive definite. The most difficult regions in mixture phase envelopes are in the vicinity of singularities: critical points for multiphase flash calculations, convergence locus for negative flashes [3], the stability test limit locus (STLL) [3–5] (or the "shadow curve" [6]) for stability analysis. Near these loci, algorithms either become extremely slow of have difficulties to converge. In the case of a too early switch, the Newton step is rejected and the calculations are switched back to SSI iterations. Sometimes a very large number of SSI iterations are necessary before the final switch to Newton iterations very close to singularities. This convergence behavior suggested us to investigate how Trust-Region methods behave in such situations.

Restricted-step methods or Trust-Region methods were first suggested by Levenberg [7] and Marquardt [8] to solve nonlinear least-squares problems. They are often put in comparison with line search techniques, and they have seen considerable improvements in the past thirty years. The first algorithms were designed to small

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systems (Hebden [9], Gill and Murray [10,11], Gay [12], Moré and Sorensen [13,14]). Then, a second branch of Trust-Region methods started to see developments since the improvements in computer science enabled to deal with bigger problems: the method based on high dimension problems, like the conjugate-gradients or generalized Lanczos-Trust-Region algorithms (Steihaug [15], Shultz et al. [16], Byrd et al. [17]). Except when dealing with a high number of components, this category is not suited for phase equilibrium calculations.

The first to introduce a Trust-Region method for equilibrium flash calculations were Nghiem et al. [18]. They applied Powel's Dogleg method to the two-phase flash calculations. The same method was then used by Lucia and Liu [19]. The dogleg method is a linear combination between a Cauchy step and Newton method. Nghiem et al. [18] adapted this method as a linear combination between the SSI and Newton iterations; the method fails when the Hessian is not positive definite. Mehra et al. [20] extended this method to multiphase equilibrium calculations.

Michelsen [21,22] addressed the problem of non-positive definite Hessians (revealed during decomposition) in phase equilibrium calculations and suggested the use of Trust-Region methods. If the Hessian matrix $\mathbf{H}$ is not positive definite, it is corrected by adding a diagonal element, that is, $\mathbf{H}+\lambda\mathbf{I}$. Then some other authors have been investigating the Trust-Region methods in phase equilibrium calculations: Trangenstein [23] reported minimization with linear constraints for phase stability and multiphase flash. Kaul and Thrasher [24] used a Trust-Region procedure similar to Hebden [9] for two-phase equilibrium flash calculations using a set of reduced variables. Pan and Firoozabadi [25] also used a Trust-Region method; however, there are certain difficulties in combining the Trust-Region approach with reduction methods.

Lucia et al. [26] developed a Trust-Region method extending the Powell dogleg strategy to the complex domain; this method was used by Gow et al. [27] to model the VLE of binary refrigerant mixtures. Lucia and Yang [28] used a Trust-Region method to calculate downhill directions in terrain global methods; these methods were used to model the complex phase behavior of normal alkane systems (Lucia et al. [29]), or within a multi-scale framework for multiphase flash calculations (Lucia et al. [30]). Alsaifi and Englezos [31] used a Trust-Region Gauss-Newton method for simultaneous stability and flash calculations with the PC-SAFT equation of state. Recently, Michelsen et al. [32] reported the use of a Trust-Region method for phase equilibrium calculations.

However, in all the developed Trust-Region methods used to solve phase equilibrium problems (flash or stability analysis), no one deals with the correction of a non-positive definite Hessian matrix. Moreover, the dogleg methods used as a linear combination between the Newton step and the Cauchy step corresponds to solving a minimization problem in a subspace of two dimensions; this gives a good approximation of the real solution, but does not give the exact minimum of the Trust-Region subproblem. In this paper, a Trust-Region method derived from Moré and Sorensen [13,14], and Conn et al. [33] is adapted and tested successfully for various phase stability analysis and multiphase flash calculations problems. This Trust-Region method works with every kind of Hessian matrix (even non-positive definite). Moreover, it calculates almost exactly the solution of the Trust-Region subproblem. The algorithm based on Moré and Sorensen [13,14] is quite old (30 years). However, one can notice that most of the recent developments of the new Trust-Region algorithms have been made for large scale problems which are more challenging; for problems with a small dimensionality, the chosen algorithm still seems to be the reference in terms of computational time. A hybrid methodology that combines SSI, Newton's method and Trust-Region steps is also proposed in this work.

The paper is structured as follows: the formulation of phase stability testing and multiphase flash calculations as minimization problems is briefly recalled, then the proposed Trust-Region method is presented in detail. The results for phase stability and multiphase flash calculations of various mixtures with complex phase envelopes and comparisons between the proposed method with Newton methods using various independent variables are presented before drawing the conclusions.

2. Equilibrium flash calculations and phase stability analysis aspects

2.1. Stability analysis

Michelsen [2] introduced the modified dimensionless tangent plane distance (TPD) function given by:

$$D_M = \left(1 - \sum_{i=1}^{nc} Y_i\right) + \sum_{i=1}^{nc} Y_i(\ln Y_i + \ln\varphi_i(\mathbf{Y}) - d_i) \tag{1}$$

where $d_i = \ln\phi_i(z) + \ln z_i$ and Y_i can be formally viewed as mole numbers.

The modified objective function has the same sign and same stationary points as the TPD function. The stability analysis problem consists in minimizing the modified TPD function. In many applications, the computational time is critical (reservoir simulations for example), thus global optimization (which is too costly) cannot be efficiently used. The standard approach is to use local optimization algorithms over different specific initial guesses. The most common initial guesses come from Wilson relation [34], and use the two-sided initialization (Michelsen [2]): $Y_i^{(0)} = z_i K_i$ (for liquid phase stability) and $Y_i^{(0)} = z_i/K_i$ (for vapor phase stability).

The minimization problem can be solved using different sets of independent variables. Using the mole numbers Y_i as the dependent variable, the gradient is given by:

$$g_i = \frac{\partial D_M}{\partial Y_i} = \ln\ Y_i + \ln\varphi_i - d_i; \quad i = 1, nc \tag{2}$$

From $\mathbf{g}(\mathbf{Y}) = 0$, the iteration equation of the SSI method (Michelsen [2]) is

$$\ln\ Y_i = d_i - \ln\ \varphi_i(\mathbf{Y}) \tag{3}$$

The SSI first order method is extremely robust but can be extremely slow as singularities are approached.

A Newton step can be carried out to update Y_i

$$\mathbf{H}\Delta\mathbf{Y} = -\mathbf{g} \tag{4}$$

with

$$H_{ij} = \frac{\partial^2 D_M}{\partial Y_i \partial Y_j} = \frac{\partial g_i}{\partial Y_j} = \frac{\delta_{ij}}{Y_i} + \frac{\partial \ln\ \varphi_i}{\partial Y_j}; \quad i, j = 1, nc \tag{5}$$

Michelsen [2] proposed the independent variables $\alpha_i = 2\sqrt{Y_i}$ for the minimization of the modified TPD function. In this case, the gradient is given by

$$\bar{g}_i = \frac{\partial D_M}{\partial \alpha_i} = g_i\sqrt{Y_i} \tag{6}$$

and the Hessian matrix is

$$\bar{H}_{ij} = \frac{\partial^2 D_M}{\partial \alpha_i \partial \alpha_j} = \delta_{ij} + \frac{1}{4}\alpha_i\alpha_j\frac{\partial \ln\varphi_i}{\partial Y_j} + \frac{1}{2}\delta_{ij}\bar{g}_i \tag{7}$$

where the second term corresponds to a generally low effective rank matrix and the last term vanishes at the solution.

Usually a switch is performed from the first- to the second-order method; this takes advantage from the strengths and avoids disadvantages of each method.