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Rapid phase stability calculations in fluid flow simulation using simple discriminating functions

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ABSTRACT

This paper presents a new phase stability method that is applicable when repeated phase behavior calculations are needed as it is the case with multiphase fluid flow compositional simulation in upstream petroleum engineering. Two discriminating functions act as classifiers in such a way that a positive value of one of the two functions determines the stability state of the mixture. The two functions are generated off line, prior to the simulation, and their expressions are very simple so that they can be evaluated rapidly in a non-iterative way for every discretization block and at each timestep during the simulation. The CPU time required for phase stability calculations is dramatically reduced while still obtaining correct classification results corresponding to the global minimum of the system Gibbs energy function. The method can be applied to any chemical engineering problem where the class of several objects needs to be determined repeatedly and quickly.

1. Introduction

Upstream petroleum engineering focuses on modeling the flow of hydrocarbons from the reservoir up to the sales point. These models are used subsequently to design the production facilities and select the operating conditions so as to maximize production at minimum field development cost. As flow is considered both within the reservoir, the production wells and the surface or seabed manifolds such models incorporate fluid flow calculations in the porous medium and in pipelines of various configurations (Floquet et al., 2009). The solution of the continuity, momentum and energy equations requires fluid properties such as density, compressibility, viscosity and enthalpy. However, reservoir fluids are complex mixtures of thousands of components and they may appear in multiphase equilibrium thus rendering compositional fluid flow simulation as a complex computational task.

Today, computers capabilities allow for the detailed numerical solution of the flow equations using very fine space grids and time discretization. Current practice is to simulate various complex production scenaria for which thermodynamic properties are calculated by means of cubic EoS models (Michelsen and Mollerup, 2004). Despite the simplicity of those models, phase behavior calculations such as identification of phase stability, determination of the phase split and calculation of the equilibrium phase properties, still consume a considerable part of the total CPU time due to the complexity of the utilized algorithms and the need to repeat them for each discretization block and timestep. This discourages operators from employing thermodynamically advanced but mathematically more complex EoS models which could capture more accurately fluid thermodynamics. Nevertheless, the utilization of advanced EoS models is a prerequisite when flow assurance issues are considered such as precipitation of asphaltenes, water chemistry, wax and hydrate formation (Subramanian, 2016; Sloan, 1990).

To determine at each discretization block and at each timestep whether the reservoir fluid appears in single phase or if two or more phases coexist in equilibrium, a phase stability calculation needs to be run (Michelsen, 1982a). If the fluid proves to be unstable a phase split calculation (Michelsen, 1982b) follows to determine the quantity and properties of the equilibrium phases. The thermodynamically rigorous approach to both problems involves the minimization of the Gibbs energy function given each block's overall composition $\mathbf{z}$, prevailing pressure p and temperature T. Although standalone phase split calculations are more complex and difficult to converge than the phase stability ones, the latter still consume a significant part of the total CPU time when flow simulation is concerned due to several reasons. Firstly, stability calculations are run always for each block and for all timesteps whereas phase split is needed only when instability occurs. For example, when dealing with undersaturated reservoirs phase split calculations might be fully skipped throughout the simulation. Secondly, phase split calculations are usually initialized to the solution of the same block at the previous timestep or a variant of that

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(e.g. Rasmussen et al., 2006), which in most cases guarantees very fast convergence, whereas phase stability calculations are initialized by correlations of limited accuracy (Whitson and Brule, 2000). Additionally, when stability calculations in the vicinity of the stability test limit locus are considered, the number of iterations may increase dramatically (Nichita et al., 2007). Moreover, to ensure convergence to the global minimum of the system energy function and avoid missing possible instability, the phase stability algorithm needs to be sophisticated enough. Clearly, both reliability and speed of the stability algorithm are issues of major importance in a simulation run.

Reliable phase stability methods address the lack of convexity of the Gibbs energy function by focusing at its global minimum using a wide variety of approaches such as homotopy continuation (Jalali et al., 2008), interval Newton methods (Staudt et al., 2013), tunneling methods (Nichita et al., 2002) and simulated annealing (Pan and Firoozabadi, 1998). Admittedly, all the above methods are computationally very expensive. Nevertheless, as opposed to standalone calculations, alternative methods might be utilized when repeated stability tests need to be run for potential phases that can be described by a fixed EoS model, as it is the case with compositional reservoir models, pipeline flow and separation process simulations. Such methods may require some extra time prior to the simulation in order to be setup but they perform significantly faster during the simulation. For example, lumping the reservoir fluid components to a smaller number of pseudo-components while preserving as much as possible the main characteristics of the Gibbs energy surface is a standard procedure (Whitson and Brule, 2000). Although several attempts might be required to achieve the best possible modification of the EoS model the reduced dimensionality of the lumped model is expected to accelerate calculations. For the case of cubic EoS models combined to the Van der Waals mixing rules, reduction methods (Hendricks and Van Bergen, 1992; Firoozabadi and Pan, 2002; Gaganis, 2013) take advantage of the limited intrinsic dimensionality of the fluid model to reduce the number of variables involved by applying spectral analysis to the binary interaction coefficients matrix. Several soft computing approaches have also been presented as alternatives to the conventional thermodynamically rigorous ones among which on-the-fly tabulation of phase behavior results so as to be used during the flow simulation (Zaydullin et al., 2014), table interpolation techniques to map the natural flow variables such as density and energy directly to pressure and temperature (Brown et al., 2016) and utilization of continuous interpolation tools such as neural networks (Schimtz et al., 2006) are the most pronounced ones.

In a recent work Gaganis and Varotsis (2014) introduced the use of classification models from the machine learning field to generate explicit, non-iterative solutions of the phase stability problem. The idea lies in developing a discriminating function $d(\mathbf{x})$, where $\mathbf{x} = [\mathbf{z}, p, T]^T$, which exhibits positive value for any stable mixture and negative value for any unstable one, the same way the classic minimum tangent plane distance criterion does. Once such a function becomes available, each discretization block during a simulation run can be classified as stable or unstable significantly faster than running iterative calculations simply by evaluating the sign of $d(\mathbf{x})$. To honor continuity $d(\mathbf{x})$ needs to exhibit a zero value for every point $\mathbf{x}$ lying on the boundary that separates stable from unstable points, hence the $d(\mathbf{x}) = 0$ contour matches exactly the phase envelope. Therefore, the complexity of the $d(\mathbf{x})$ expression, hence the CPU time needed to evaluate it, depends on the shape of the phase boundary which in turn is a function of the fluid's number of components and the operating range of $\mathbf{x}$.

In this work a new classification technique is presented which relaxes the need of $d(\mathbf{x})$ to emulate exactly the phase boundary, thus allowing for great simplification of the discriminating function expression and leading to rapid phase stability determination. The classifier $d(\mathbf{x})$, the sign of which provides correct answers for both classes, is replaced by two discriminating functions $d_A(\mathbf{x})$ and $d_B(\mathbf{x})$, each one providing accurate answers for one class solely. The classifiers are defined by simple and very fast to evaluate expressions and designed so that $d_A(\mathbf{x}) > 0$ implies that mixture $\mathbf{x}$ is stable and $d_B(\mathbf{x}) > 0$ implies that it is unstable. The converse is not necessarily true, therefore correct classifications can be guaranteed only when one of the two classifiers exhibits a positive value. To minimize ambiguity, that is the occurrence of points for which both classifiers exhibit negative value, the loci of $d_A(\mathbf{x}) > 0$ and $d_B(\mathbf{x}) > 0$ need to cover as much as possible of the stable and unstable regions respectively. This way, correct classification results can be obtained rapidly for the vast majority of the discretization blocks during the simulation at the cost of the evaluation of one of the two simple classifiers solely. As it will be shown, that cost is just a small fraction of the CPU time required by the conventional iterative approach.

The paper is structured as follows: Section 2 discusses the equivalence between the thermodynamically rigorous iterative approach and the use of explicit discriminating functions in phase stability calculations. Section 3 presents the properties that the proposed classifiers need to exhibit and Section 4 sets up the mathematical program to generate them. Section 5 addresses several computational issues. A set of examples demonstrates the efficiency of the method in Section 6 followed by the conclusions.

2. Discriminating functions equivalence to the phase stability problem

Currently, stability of a mixture of composition $\mathbf{z}$ at pressure p and at temperature T is determined by means of Michelsen's criterion (1982a) according to which the mixture will split in two or more phases only if

$$TPD(\mathbf{z}, p, T, \boldsymbol{y}) < 0 \tag{1}$$

or

$$TPD(\mathbf{z}, p, T, \boldsymbol{y}) = 0, \boldsymbol{y} \neq \boldsymbol{z} \tag{2}$$

for some composition $\mathbf{y}$ an infinitesimal quantity of which forms a second phase. The tangent plane distance is defined as the Gibbs energy difference between the single phase and the two phase mixtures, i.e. $TPD = g_{mix}(\mathbf{z}, \mathbf{y}, p, T) - g(\mathbf{z}, p, T)$. Eq. (2) corresponds to an incipient equilibrium second phase while a stable phase exhibits $TPD(\mathbf{z}, p, T, \mathbf{y}) > 0$ for any composition $\mathbf{y}$. Instead of searching exhaustively the whole compositional space for compositions $\mathbf{y}$ that might satisfy Eqs. (1) or (2) Michelsen suggested the utilization of optimization to compute the minimizers

$$\mathbf{y}_{\min} = \underbrace{arg\,\min}_{\mathbf{y}} \left\{ TPD(\mathbf{z}, p, T, \mathbf{y}) \right\} \tag{3}$$

and the evaluation of the sign of $TPD_{\min}$ at $\mathbf{y}_{\min}$. Nevertheless, the stationary points of the significantly non-convex TPD surface can only be found by means of CPU time expensive iterative methods such as the Newton or the Successive Substitution ones. Moreover, being trapped to a local minimum is always an issue thus introducing the need of global optimization methods or of repeated trials using various initialization schemes (Muller and Marquardt, 1997). Clearly, being able to compute $TPD_{\min}(\mathbf{z}, p, T)$ rapidly (in fact its sign is only required) by means of an explicit expression would be highly beneficial.

From a different point of view, determining the stability state of a mixture can be seen as a binary classification problem (Duda