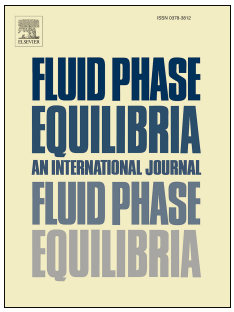
Accepted Manuscript



Extension of modified RAND to multiphase flash specifications based on state functions other than (*T*,*P*)

Duncan Paterson, Michael L. Michelsen, Wei Yan, Erling H. Stenby

PII: S0378-3812(17)30401-6

DOI: 10.1016/j.fluid.2017.10.019

Reference: FLUID 11620

To appear in: *Fluid Phase Equilibria*

Received Date: 27 June 2017

Revised Date: 6 October 2017

Accepted Date: 20 October 2017

Please cite this article as: D. Paterson, M.L. Michelsen, W. Yan, E.H. Stenby, Extension of modified RAND to multiphase flash specifications based on state functions other than (*T*,*P*), *Fluid Phase Equilibria* (2017), doi: 10.1016/j.fluid.2017.10.019.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

Extension of Modified RAND to Multiphase Flash Specifications Based on State Functions Other than (T, P)

Duncan Paterson[a], Michael L. Michelsen[b], Wei Yan[a,*], Erling H. Stenby[a]

[a] *Center for Energy Resources Engineering, Department of Chemistry, Technical University of Denmark, DK-2800 Lyngby, Denmark*
[b] *Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark*

Abstract

The recently proposed modified RAND formulation is extended from isothermal multiphase flash to several other state function based flash specifications. The obtained general formulation is applicable to chemical equilibrium although this study is focused on flash with only phase equilibrium. It is demonstrated that a common symmetric Jacobian matrix can be formulated for all of these flash specifications. Newton iteration with the common Jacobian is used to converge for the majority of cases and a Q-function maximisation with nested isothermal flash in the inner loop is used for the non-convergent exceptions. For isothermal flash with modified RAND, it can happen in rare occasions that the modified RAND step is ascending in the Gibbs energy. A correction of the step is proposed for such cases to obtain a descent direction without violating the condition used in the derivation of modified RAND. A two-phase example is used to demonstrate that the described method is suitable for (H, P), (T, V), (S, V) and (U, V) flash specifications and a four-phase case is examined in more detail for the difficult (U, V) case. Two- and three-phase examples close to critical regions are used to demonstrate the effectiveness of the correction procedure for the modified RAND step and to show that satisfactory rates of convergence are obtained.

1. Introduction

Many simulations in the oil, gas and chemical industry require the solution to the phase equilibrium problem. The classical example is the isothermal flash where composition, pressure and temperature are specified. The conventional approach to solve the isothermal flash problem involves stability analysis (Michelsen, 1982a; Baker et al., 1982) and phase split calculation (Michelsen,

*Corresponding author

Download English Version:

https://daneshyari.com/en/article/6619373

Download Persian Version:

https://daneshyari.com/article/6619373

Daneshyari.com