



# A robust algorithm for isenthalpic flash of narrow-boiling fluids



Di Zhu, Ryosuke Okuno\*

School of Petroleum Engineering, University of Alberta, Canada

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## ABSTRACT

Numerical solution of many non-isothermal reservoir flow problems requires robust isenthalpic flash. However, isenthalpic flash is challenging when the total enthalpy is sensitive to temperature, which is referred to as narrow-boiling behavior. The direct substitution (DS) algorithms proposed in the literature have convergence difficulties for narrow-boiling fluids.

This research presents a detailed analysis of the narrow-boiling behavior and its effects on the robustness of the DS algorithms. A new DS algorithm is developed that addresses the direct reason for the convergence issues associated with narrow-boiling behavior. The main focus of the research is on robust isenthalpic flash for two hydrocarbon phases, although mathematical derivations are given for a general multicomponent multiphase system. The thermodynamic model used is the Peng–Robinson equation of state.

The new DS algorithm is tested for various isenthalpic flash problems, which include the cases for which the prior DS algorithms exhibit non-convergence. Results show that the narrow-boiling behavior causes the system of equations solved in the DS algorithms to be degenerate. The degenerate equations can be robustly handled by the bisection algorithm developed in this research. Case studies demonstrate that the new DS algorithm exhibits significantly improved robustness for isenthalpic flash of narrow-boiling fluids.

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## 1. Introduction

Steam injection is a widely used method for heavy-oil recovery [1]. The steam injected releases the latent heat when it condenses into hot water at thermal fronts. Part of the heat can effectively increase the oleic phase mobility because heavy-oil viscosity is highly sensitive to temperature [2,3]. Steam-assisted gravity drainage (SAGD) is an important application of steam injection for recovery of extra-heavy oil and bitumen [4].

Flow of fluid and energy is coupled with multiphase behavior of water–hydrocarbons mixtures in steam injection. A wide variety of compounds that exist in a heavy-oil reservoir have different volatilities. Different compounds propagate differently in a reservoir during the non-isothermal recovery process. Therefore, compositional effects are important in understanding and designing steam injection. For example, thermodynamic conditions at thermal fronts are dependent on multiphase behavior of water–hydrocarbons mixtures at elevated temperatures [5]. Vaporization and condensation of light hydrocarbons, one of the main oil-recovery mechanisms in steam injection, is a consequence of the complex interaction between reservoir flow and multiphase behavior [2,6–10].

Compositional simulation of steam injection has been common practice in the oil industry, in which phase behavior is solved for based on  $K$ -value tables prepared for different temperatures and pressures [11–13]. The thermal simulation based on  $K$  values is computationally efficient and reasonably accurate in estimating reservoir processes. However, it does not capture detailed compositional effects on phase equilibria and phase properties. A more general approach to phase behavior modeling is to use a cubic equation of state (EoS) in place of  $K$ -value tables [9,14–17]. Phase behavior modeling based on an EoS is particularly important when the primary focus of flow simulation is on investigation of detailed recovery mechanisms [9,18]. Recently, Iranshahr et al. [19] presented an efficient EoS thermal simulator on the basis of phase behavior parameterization using tie-line information.

\* Corresponding author at: 3-114 Markin/CNRL Natural Resources Engineering Facility, University of Alberta, Edmonton, AB T6G 2W2, Canada. Tel.: +1 780 492 6121; fax: +1 780 492 0249.

E-mail addresses: [rokuno@ualberta.ca](mailto:rokuno@ualberta.ca), [okuno@alumni.utexas.net](mailto:okuno@alumni.utexas.net) (R. Okuno).

## Nomenclature

### Roman symbols

$a$	attraction parameter for a cubic equation of state
$A$	dimensionless attraction parameter for a cubic equation of state
$b$	covolume parameter for a cubic equation of state
$B$	dimensionless covolume parameter for a cubic equation of state
$C$	constant defined for temperature oscillation check
$C_{Pj}$	heat capacity of phase $j$
$\underline{C}_{Pi}^0$	coefficients of component $i$ defined in Eq. (17)
$\underline{f}$	vector consisting of $N_C$ residuals of the fugacity equations
$f_i$	residual of the fugacity equations defined in Eq. (9)
$f_{ij}$	fugacity of component $i$ in phase $j$ , or residual of the fugacity equations defined in Eq. (5)
$f_o$	function defined for temperature oscillation check
$g_j$	residuals of material balance equations ( $j = 1, 2, \dots, N_p - 1$ )
$g_{N_p}$	residual of the enthalpy constraint
$\underline{G}$	molar Gibbs free energy
$H$	enthalpy
$\underline{H}$	molar enthalpy
$k_{ij}$	binary interaction parameter between components $i$ and $j$
$\underline{K}$	vector consisting of $N_C$ $K$ values
$K_i$	$K$ value of component $i$ for a two-phase system defined in Eq. (10)
$K_{ij}$	$K$ value of component $i$ in phase $j$
$L$	liquid phase
$N_C$	number of components
$N_p$	number of phases
$P$	pressure
$P_C$	critical pressure
$R$	universal gas constant
$\underline{S}$	molar entropy
$T$	temperature
$T_C$	critical temperature
$T_0$	273.15 K defined in Eq. (17)
$V$	vapor phase
$\underline{V}$	molar volume
$x_i$	mole fraction of component $i$ in the L phase for a L–V two-phase system
$x_{ij}$	mole fraction of component $i$ in phase $j$
$y_i$	mole fraction of component $i$ in the V phase for a L–V two-phase system
$z_i$	mole fraction of component $i$ in a mixture
$Z_j$	compressibility factor of phase $j$

### Greek symbols

$\alpha$	coefficients defined in Eq. (21)
$\beta_j$	mole fraction of phase $j$
$\varepsilon$	convergence criterion (e.g., $10^{-10}$ )
$\varepsilon_o$	constant used for temperature oscillation check
$\varphi_{ij}$	fugacity coefficient of component $i$ in phase $j$
$\omega$	acentric factor

### Subscripts

C	critical property
D	dimensionless property
$i$	component index
$j$	phase index
m	mixture
ref	reference value
spec	specified value

### Superscripts

dep	departure
IG	ideal gas
IGM	ideal gas mixture
$k$	index for iteration steps
L	lower bound
t	total property

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