Draft Technical Documentation

# Description of the Thermal GPRS

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# 1 Introduction

In this document, we discuss the description of the standard hydrodynamics simulator GPRS (General Purpose Research Simulator). We also discuss the extension of the standard simulator to a thermal one.

## 1.1 General physical model

The standard mass balance equations of a system containing $n_c$ components can be presented as follows:

$$F_c = \frac{\partial}{\partial t}\left(\phi \sum_p x_{c,p}\rho_p S_p\right) - \text{div}\sum_p x_{c,p}\rho_p \mathbf{u}_p + \sum_p x_{c,p}\rho_p q_p, \quad c = 1,\ldots,n_c \tag{1.1}$$

Darcy law is used to describe the flow of all three phases (oil, water and gas):

$$\mathbf{u}_p = \left(\mathbf{k}\frac{k_{rp}}{\mu_p}(\nabla p_p - \gamma_p \nabla D)\right), \quad p = o,w,g \tag{1.2}$$

In order to take into account the thermal processes, we also need to add the energy equation to the system:

$$F_e = \frac{\partial}{\partial t}\left(\phi\left(\sum_p U_p\rho_p S_p\right) + (1-\phi)U_R\right) - \text{div}\left(\sum_p H_p\rho_p \mathbf{u}_p\right) - \text{div}\left(\kappa\nabla T\right) + \left(\sum_p H_p\rho_p q_p\right) \tag{1.3}$$

The primary variables for the black-oil and compositional models are:

- $p = p_g(t,xyz)$ – gas phase pressure,

- $T = T(t,xyz)$ – temperature,

- $S_p = S_p(t,xyz)$ – phase $p$, $p = o,w$ saturation,

The black-oil set of variables differs from the compositional one in the mass fractions. In the black-oil model, mass fractions are functions of primary variables

$$x_{c,P} = x_{c,P}(p,T,\mathbf{S})$$

In the compositional case, we use $x_c = x_{c,o}$ and $y_c = x_{c,g}$ as base variables.
Other unknowns can be presented as functions of primary variables:

- $S_g = S_g(\mathbf{S})$ – gas saturation,

- $\phi = \phi(p,xyz)$ – porosity,

- $\mathbf{k} = \mathbf{k}(p,xyz)$ – permeability tensor,

- $p_o = p - P_{cgo}(S_g)$ – oil phase pressure,

- $p_w = p - P_{cgo}(S_g) - P_{cwo}(S_w)$ – water phase pressure,

- $\rho_p = \rho_p(p,T,\mathbf{S})$ – phase molar density,

- $k_{rp} = k_{rp}(T,\mathbf{S})$ – phase relative permeability,

- $\mu_p = \mu_p(p,T,\mathbf{S})$ – phase viscosity,

- $\gamma_p = \rho'_p g$ – vertical pressure gradient,

- $D = D(x, y, z)$ – vertical depth vector (up-down oriented),

- $q_p = q_p(p, \mathbf{S}, t, x, y, z)$ – reduced source of phase,

- $U_p = U_p(p, T, \mathbf{S})$ – phase internal energy,

- $U_R = U_R(p, T)$ – rock internal energy,

- $H_p = H_p(p, T, \mathbf{S})$ – phase enthalpy,

- $\kappa = \kappa(p, T)$ – thermal conduction,

After standard finite-volume discretization on a rectangular mesh we obtain

$$
\begin{aligned}
F_c &= \frac{\partial}{\partial t} V \left[ \phi \left( \sum_p x_{c,p} \rho_p S_p \right) \right] - \sum_l \left( \sum_p x_{cp}^l \rho_p^l \Gamma_p^l \Delta \Phi_p^l \right) + \sum_p \rho_p x_{cp} Q_p, \quad (1.4) \\
&\quad c = 1, \dots, n_c \\
F_e &= \frac{\partial}{\partial t} V \left[ \phi \sum_p S_p \rho_p U_p + (1 - \phi) U_R \right] - \sum_l \left( \sum_p H_p^l \rho_p^l \Gamma_p^l \Delta \Phi_p^l + \Gamma_c^l \Delta T^l \right) + \left( \sum_p \rho_p H_p Q_p \right) \quad (1.5)
\end{aligned}
$$

here upper index $l$ represents all quantities defined at the interface between connected cells. All indexes for grid cells are missing.

During discretization we defined additional functions:

- $V = V(x, y, z)$ – cell volume,

- $\Gamma_p^l = \Gamma^l \dfrac{k_{rp}^l}{\mu_p^l}$ – phase transmissibility,

- $\Gamma^l = \Gamma^l(x, y, z)$ – constant part of transmissibility,

- $\Delta \Phi_p^l = p_p^a - p_p^b - \gamma_p(D^a - D^b)$ – difference in potential between blocks $a$ and $b$ (from left and from right of interface $l$),

- $\Gamma_c^l = \Gamma^l \kappa$ – thermal transmissibility,

- $\Delta T = T^a - T^b$ – difference in potential between blocks $a$ and $b$,

- $Q_p = q_p V$ – volumetric source of phase.

## 1.2 Black-oil model

The current implementation of GPRS includes some simplifications in terms of function description. We use the same system of equations described as in (1.4)- (1.5).

GPRS uses the same set of primary variables as the general black-oil description (Type A variables, see Hui Cao's thesis for explanation between Type A and Type B set of variables):

- $p = p_g(t, xyz)$ – gas phase pressure,

- $T = T(t, xyz)$ – temperature,

- $S_p = S_p(t,xyz)$ – phase $p$, $p = o,w$ saturation,

There are some differences for the description of the functions:

- $S_g = S_g(\mathbf{S})$ – gas saturation,

- $\phi = \phi(p,xyz)$ – porosity,

- $\mathbf{k} = \mathbf{k}(xyz)$ – permeability tensor,

- $p_o = p - P_{cgo}(S_g)$ – oil phase pressure,

- $p_w = p - P_{cgo}(S_g) - P_{cwo}(S_w)$ – water phase pressure,

- $x_{c,P} = x_{c,P}(p,T)$ – molar concentrations,

- $\rho_p = \rho_p(p,T)$ – phase molar density,

- $k_{rp} = k_{rp}(T,\mathbf{S})$ – phase relative permeability,

- $\mu_p = \mu_p(p,T)$ – phase viscosity,

- $\gamma_p = \rho'_p g$ – vertical pressure gradient,

- $D = D(x,y,z)$ – vertical depth vector (up-down oriented),

- $q_p = q_p(p,\mathbf{S},t,x,y,z)$ – reduced source of phase,

- $U_p = U_p(p,T)$ – phase internal energy,

- $U_R = U_R(p,T)$ – rock internal energy,

- $H_p = H_p(p,T)$ – phase enthalpy,

- $\kappa = \text{const}$ – thermal conduction,

## 1.3 Compositional model

The system of equations for the compositional model is presented in the standard form in GPRS(1.4)- (1.5).
The base compositional description in GPRS uses the following set of variables

- $p = p_g(t,xyz)$ – gas phase pressure,

- $T = T(t,xyz)$ – temperature,

- $S_p = S_p(t,xyz)$ – phase $p$, $p = o,w$ saturation,

- $x_c = x_c(t,xyz)$ – liquid phase concentration for each component $c$,

- $y_c = y_c(t,xyz)$ – gas phase concentration for each component $c$.

In the compositional model, we also change the way functions are defined

- $S_g = S_g(\mathbf{S})$ – gas saturation,

- $\phi = \phi(p,xyz)$ – porosity,

- $\mathbf{k} = \mathbf{k}(xyz)$ – permeability tensor,

- $p_o = p - P_{cgo}(S_g)$ – oil phase pressure,

- $p_w = p - P_{cgo}(S_g) - P_{cwo}(S_w)$ – water phase pressure,

- $x_{c,w} = x_{c,w}(p,T)$ – molar concentration,

- $\rho_w = \rho_w(p,T)$ – water phase molar density,

- $\rho_o = \rho_o(p,T,\mathbf{x})$ – oil phase molar density,

- $\rho_g = \rho_g(p,T,\mathbf{y})$ – gas phase molar density,

- $k_{rp} = k_{rp}(T,\mathbf{S})$ – phase relative permeability,

- $\mu_w = \mu_w(p,T)$ – water phase viscosity,

- $\mu_p = \mu_o(p,T,\mathbf{x})$ – oil phase viscosity,

- $\mu_p = \mu_g(p,T,\mathbf{y})$ – gas phase viscosity,

- $\gamma_p = \rho'_p g$ – vertical pressure gradient,

- $D = D(x,y,z)$ – vertical depth vector (up-down oriented),

- $q_p = q_p(p,\mathbf{S},t,x,y,z)$ – reduced source of phase,

- $U_w = U_w(p,T)$ – phase internal energy,

- $U_o = U_o(p,T,\mathbf{x})$ – phase internal energy,

- $U_g = U_g(p,T,\mathbf{y})$ – phase internal energy,

- $U_R = U_R(p,T)$ – rock internal energy,

- $H_w = H_w(p,T)$ – phase enthalpy,

- $H_o = H_o(p,T,\mathbf{x})$ – phase enthalpy,

- $H_g = H_g(p,T,\mathbf{y})$ – phase enthalpy,

- $\kappa = \mathrm{const}$ – thermal conduction,

# 2 Black-oil model formulation

In order to find the solution of the black-oil problem, we need to solve the system of non-linear equations $F(X) = 0$ where the vector of unknown variables is $X = \{p, T, S_w, S_o\}$ and the equations are taken from (1.4)- (1.5). The gas saturation $S_g$ is usually represented as a function of the other two saturations

$$S_g(S_o, S_w) \quad = \quad 1 - S_o - S_w \tag{2.1}$$

We use Newton method to linearize the system of equations

$$J\delta X = -F \tag{2.2}$$

## 2.1 General black-oil model

In this section, we use the general black-oil model without any explicit assumptions (except standard black-oil assumption, see 1.2). To obtain the Jacobian, we need to completely derive our system:

$$
\begin{aligned}
\frac{\partial F_c}{\partial p} \quad = \quad & V\left[\frac{\partial \phi}{\partial p}\sum_p S_p \rho_p x_{cp} + \phi \sum_p S_p\left(\frac{\partial \rho_p}{\partial p}x_{cp} + \rho_p \frac{\partial x_{cp}}{\partial p}\right)\right] \\
& - \tau \sum_l \sum_p \left(\frac{\partial x_{cp}}{\partial p}^l \rho_p^l \Gamma_p^l \Delta\Phi_p^l + x_{cp}^l \frac{\partial \rho_p^l}{\partial p}\Gamma_p^l \Delta\Phi_p^l + x_{cp}^l \rho_p^l \frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + x_{cp}^l \rho_p^l \Gamma_p^l \frac{\partial \Delta\Phi_p^l}{\partial p}\right) \\
& + \tau \sum_p \left(\frac{\partial \rho_p}{\partial p}x_{cp}Q_p + \rho_p \frac{\partial x_{cp}}{\partial p}Q_p + \rho_p x_{cp}\frac{\partial Q_p}{\partial p}\right), \quad c = 1, \dots, n_c
\end{aligned} \tag{2.3}
$$

It is important to notice that we calculate the derivatives for each component of vector **p** in each grid cell which means that our description of derivatives is

$$\frac{\partial F_c}{\partial p} = \frac{\partial F_c^i}{\partial p^j}$$

where $i$ and $j$ are numbers of grid cells.

Similarly, we can calculate pressure derivatives for the other equations

$$
\begin{aligned}
\frac{\partial F_e}{\partial p} \quad = \quad & V\left[\frac{\partial \phi}{\partial p}\left(\sum_p S_p \rho_p U_p - U_R\right) + \phi \sum_p \left(S_p \frac{\partial \rho_p}{\partial p}U_p + S_p \rho_p \frac{\partial U_p}{\partial p}\right) + (1-\phi)\frac{\partial U_R}{\partial p}\right] \\
& - \tau \sum_l \sum_p \left(\frac{\partial H_p^l}{\partial p}\rho_p^l \Gamma_p^l \Delta\Phi_p^l + H_p^l \frac{\partial \rho_p^l}{\partial p}\Gamma_p^l \Delta\Phi_p^l + H_p^l \rho_p^l \frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + H_p^l \rho_p^l \Gamma_p^l \frac{\partial \Delta\Phi_p^l}{\partial p} + \frac{\partial \Gamma_c^l}{\partial p}\Delta T^l\right) \\
& + \tau \sum_p \left(\frac{\partial \rho_p}{\partial p}H_p Q_p + \rho_p \frac{\partial H_p}{\partial p}Q_p + \rho_p H_p \frac{\partial Q_p}{\partial p}\right)
\end{aligned} \tag{2.4}
$$

Then we calculate the saturation $S_{p'}$ derivatives

$$\frac{\partial F_c}{\partial S_{p'}} = V\Big[\phi\sum_p\Big(\frac{\partial S_p}{\partial S_{p'}}\rho_p x_{cp}+S_p\frac{\partial \rho_p}{\partial S_{p'}}x_{cp}+S_p\rho_p\frac{\partial x_{cp}}{\partial S_{p'}}\Big)\Big] \tag{2.5}$$

$$-\ \tau\sum_l\sum_p\Big(\frac{\partial x_{cp}}{\partial S_{p'}}^l\rho_p^l\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\frac{\partial\rho_p^l}{\partial S_{p'}}\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\rho_p^l\frac{\partial\Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l+x_{cp}^l\rho_p^l\Gamma_p^l\frac{\partial\Delta\Phi_p^l}{\partial S_{p'}}\Big)$$

$$+\ \tau\sum_p\Big(\frac{\partial\rho_p}{\partial S_{p'}}x_{cp}Q_p+\rho_p\frac{\partial x_{cp}}{\partial S_{p'}}Q_p+\rho_p x_{cp}\frac{\partial Q_p}{\partial S_{p'}}\Big),\quad c=1,\ldots,n_c$$

$$\frac{\partial F_e}{\partial S_{p'}} = V\Big[\phi\sum_p\Big(\frac{\partial S_p}{\partial S_{p'}}\rho_p U_p+S_p\frac{\partial\rho_p}{\partial S_{p'}}U_p+S_p\rho_p\frac{\partial U_p}{\partial S_{p'}}\Big)\Big] \tag{2.6}$$

$$-\ \tau\sum_l\sum_p\Big(\frac{\partial H_p^l}{\partial S_{p'}}\rho_p^l\Gamma_p^l\Delta\Phi_p^l+H_p^l\frac{\partial\rho_p^l}{\partial S_{p'}}\Gamma_p^l\Delta\Phi_p^l+H_p^l\rho_p^l\frac{\partial\Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l+H_p^l\rho_p^l\Gamma_p^l\frac{\partial\Delta\Phi_p^l}{\partial S_{p'}}+\frac{\partial\Gamma_c^l}{\partial S_{p'}}\Delta T^l\Big)$$

$$+\ \tau\sum_p\Big(\frac{\partial\rho_p}{\partial S_{p'}}H_p Q_p+\rho_p\frac{\partial H_p}{\partial S_{p'}}Q_p+\rho_p H_p\frac{\partial Q_p}{\partial S_{p'}}\Big)$$

Finally we need the temperature $T$ derivatives

$$\frac{\partial F_c}{\partial T} = V\Big[\phi\sum_p S_p\Big(\frac{\partial\rho_p}{\partial T}x_{cp}+\rho_p\frac{\partial x_{cp}}{\partial T}\Big)\Big] \tag{2.7}$$

$$-\ \tau\sum_l\sum_p\Big(\frac{\partial x_{cp}}{\partial T}^l\rho_p^l\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\frac{\partial\rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\rho_p^l\frac{\partial\Gamma_p^l}{\partial T}\Delta\Phi_p^l\Big)$$

$$+\ \tau\sum_p\Big(\frac{\partial\rho_p}{\partial T}x_{cp}Q_p+\rho_p\frac{\partial x_{cp}}{\partial T}Q_p+\rho_p x_{cp}\frac{\partial Q_p}{\partial T}\Big),\quad c=1,\ldots,n_c$$

$$\frac{\partial F_e}{\partial T} = V\Big[\phi\sum_p\Big(S_p\frac{\partial\rho_p}{\partial T}U_p+S_p\rho_p\frac{\partial U_p}{\partial T}\Big)+(1-\phi)\frac{\partial U_R}{\partial T}\Big] \tag{2.8}$$

$$-\ \tau\sum_l\sum_p\Big(\frac{\partial H_p^l}{\partial T}\rho_p^l\Gamma_p^l\Delta\Phi_p^l+H_p^l\frac{\partial\rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l+H_p^l\rho_p^l\frac{\partial\Gamma_p^l}{\partial T}\Delta\Phi_p^l$$

$$+\ \frac{\partial\Gamma_c^l}{\partial T}\Delta T^l+\Gamma_c^l\frac{\partial\Delta T^l}{\partial T}\Big)+\tau\sum_p\Big(\frac{\partial\rho_p}{\partial T}H_p Q_p+\rho_p\frac{\partial H_p}{\partial T}Q_p+\rho_p H_p\frac{\partial Q_p}{\partial T}\Big)$$

## 2.2 GPRS simplifications

Using the simplifications presented in 1.2, we can significantly simplify the Jacobian description:

$$
\begin{aligned}
\frac{\partial F_c}{\partial p} &= V\Big[\frac{\partial \phi}{\partial p}\sum_{p=o,g}S_p\rho_p x_{cp} + \phi\sum_p S_p\Big(\frac{\partial \rho_p}{\partial p}x_{cp}+\rho_p\frac{\partial x_{cp}}{\partial p}\Big)\Big] \\
&- \tau\sum_l\sum_p\Big(\frac{\partial x_{cp}}{\partial p}^l\rho_p^l\Gamma_p^l\Delta\Phi_p^l + x_{cp}^l\frac{\partial \rho_p^l}{\partial p}\Gamma_p^l\Delta\Phi_p^l + x_{cp}^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + x_{cp}^l\rho_p^l\Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial p}\Big) \\
&+ \tau\sum_{p=o,w}\Big(\frac{\partial \rho_p}{\partial p}x_{cp}Q_p + \rho_p\frac{\partial x_{cp}}{\partial p}Q_p + \rho_p x_{cp}\frac{\partial Q_p}{\partial p}\Big), \quad c=1,\dots,n_h
\end{aligned} \tag{2.9}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial p} &= V\Big[\frac{\partial \phi}{\partial p}\Big(\sum_p S_p\rho_p U_p - U_R\Big) + \phi\sum_p\Big(S_p\frac{\partial \rho_p}{\partial p}U_p + S_p\rho_p\frac{\partial U_p}{\partial p}\Big) + (1-\phi)\frac{\partial U_R}{\partial p}\Big] \\
&- \tau\sum_l\sum_p\Big(\frac{\partial H_p^l}{\partial p}\rho_p^l\Gamma_p^l\Delta\Phi_p^l + H_p^l\frac{\partial \rho_p^l}{\partial p}\Gamma_p^l\Delta\Phi_p^l + H_p^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + H_p^l\rho_p^l\Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial p}\Big) \\
&+ \tau\sum_p\Big(\frac{\partial \rho_p}{\partial p}H_pQ_p + \rho_p\frac{\partial H_p}{\partial p}Q_p + \rho_p H_p\frac{\partial Q_p}{\partial p}\Big)
\end{aligned} \tag{2.10}
$$

Then we calculate the saturation $S_{p'}$ derivatives

$$
\begin{aligned}
\frac{\partial F_c}{\partial S_{p'}} &= V\Big[\phi\sum_p\Big(\frac{\partial S_p}{\partial S_{p'}}\rho_p x_{cp}\Big)\Big] - \tau\sum_l\sum_p\Big(x_{cp}^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l + x_{cp}^l\rho_p^l\Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial S_{p'}}\Big) \\
&+ \tau\sum_p\Big(\rho_p x_{cp}\frac{\partial Q_p}{\partial S_{p'}}\Big), \quad c=1,\dots,n_h
\end{aligned} \tag{2.11}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial S_{p'}} &= V\Big[\phi\sum_p\Big(\frac{\partial S_p}{\partial S_{p'}}\rho_p U_p\Big)\Big] - \tau\sum_l\sum_p\Big(H_p^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l + H_p^l\rho_p^l\Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial S_{p'}}\Big) \\
&+ \tau\sum_p\Big(\rho_p H_p\frac{\partial Q_p}{\partial S_{p'}}\Big)
\end{aligned} \tag{2.12}
$$

And finally we simplify the temperature $T$ derivatives

$$
\begin{aligned}
\frac{\partial F_c}{\partial T} &= V\Big[\phi\sum_p S_p\Big(\frac{\partial \rho_p}{\partial T}x_{cp} + \rho_p\frac{\partial x_{cp}}{\partial T}\Big)\Big] \\
&- \tau\sum_l\sum_p\Big(\frac{\partial x_{cp}}{\partial T}^l\rho_p^l\Gamma_p^l\Delta\Phi_p^l + x_{cp}^l\frac{\partial \rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l + x_{cp}^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial T}\Delta\Phi_p^l\Big) \\
&+ \tau\sum_p\Big(\frac{\partial \rho_p}{\partial T}x_{cp}Q_p + \rho_p\frac{\partial x_{cp}}{\partial T}Q_p + \rho_p x_{cp}\frac{\partial Q_p}{\partial T}\Big), \quad c=1,\dots,n_h
\end{aligned} \tag{2.13}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial T} &= V\Big[\phi\sum_p\Big(S_p\frac{\partial \rho_p}{\partial T}U_p + S_p\rho_p\frac{\partial U_p}{\partial T}\Big) + (1-\phi)\frac{\partial U_R}{\partial T}\Big] \\
&- \tau\sum_l\sum_p\Big(\frac{\partial H_p^l}{\partial T}\rho_p^l\Gamma_p^l\Delta\Phi_p^l + H_p^l\frac{\partial \rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l + H_p^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial T}\Delta\Phi_p^l + \Gamma_c^l\frac{\partial \Delta T^l}{\partial T}\Big) \\
&+ \tau\sum_p\Big(\frac{\partial \rho_p}{\partial T}H_pQ_p + \rho_p\frac{\partial H_p}{\partial T}Q_p + \rho_p H_p\frac{\partial Q_p}{\partial T}\Big)
\end{aligned} \tag{2.14}
$$

## 2.3 Black-oil correlations used in GPRS

In this section, we introduce some functions and correlations used in the description of the thermal black-oil model implemented in GPRS

$$\phi = \phi_{ref}\left[1 + c_R(p - p_{ref})\right],$$ (2.15)

$\phi_{\text{ref}}$    is the porosity at the reference pressure,

$p_{\text{ref}}$    is the reference pressure,

$c_R$    is the rock compressibility.

$$U_R = C_R(T - T_{\text{ref}}),$$ (2.16)

$T_{\text{ref}}$    is the reference temperature,

$C_R$    is rock specific heat capacity,

$$U_p = C_p(T)(T - T_{ref}),$$ (2.17)

$T_{\text{ref}}$    is the reference temperature,

$C_p$    is fluid specific heat capacity,

$$\rho_p(p,T) = \rho_p^T(p_{ref},T)\frac{\rho_p^p(p)}{\rho_p^p(p_{ref})},$$ (2.18)

$p_{\text{ref}}$    is the reference pressure,

$\rho_p$    $= \rho_p^{SC}b_p,$

$b_p$    is interpolated from PVT tables for $p$ and $T$,

$$\mu_p(p,T) = \mu_p^T(p_{ref},T)\frac{\mu_p^p(p)}{\mu_p^p(p_{ref})},$$ (2.19)

$p_{\text{ref}}$    is the reference pressure,

$\mu_p$    is interpolated from PVT tables for $p$ and $T$,

We also introduce some additional functions:

$$S_g = 1 - S_o - S_w \tag{2.20}$$

$$x_{c,p} = \begin{cases} x_{w,w} = 1, & x_{o,w} = 0, & x_{g,w} = 0 \\ x_{w,o} = 0, & x_{o,o} = \dfrac{\rho_o^{sc}}{\rho_o^{sc} + R_{so}\rho_g^{sc}}, & x_{g,o} = 1 - x_{o,o} \\ x_{w,g} = 0, & x_{o,g} = 0, & x_{g,g} = 1 \end{cases} \tag{2.21}$$

$$k_{rp} = k_{rp}(T, \mathbf{S}) \tag{2.22}$$

$$\Gamma_p = \Gamma \frac{k_{rp}}{\mu_p}, \quad p = o, g, w \tag{2.23}$$

$$\Delta \Phi_p = \begin{cases} p^a - p^b - \overline{\rho_o} g (D^a - D^b) - (P_{cgo}^a - P_{cgo}^b), & p = o \\ p^a - p^b - \overline{\rho_w} g (D^a - D^b) - (P_{cgo}^a + P_{cwo}^a - P_{cgo}^b - P_{cwo}^b), & p = w \\ p^a - p^b - \overline{\rho_g} g (D^a - D^b), & p = g \end{cases} \tag{2.24}$$

$$Q_p = -\Gamma^w \frac{k_{rp}}{\mu_p \left(\log(r_0/r_w) + s\right)} (p - p_{BH}), \quad p = o, g, w \tag{2.25}$$

$$H_p = U_p + \frac{p_p}{\rho_p} \tag{2.26}$$

## 2.4  Derivatives calculated in GPRS

In order to calculate the Jacobian for Newton method, we need to define the following pressure derivatives

$$\frac{\partial \phi}{\partial p} = \phi_{\text{ref}} c_R \tag{2.27}$$

$$\frac{\partial \rho_p}{\partial p} = \frac{\rho_p^p(p)}{\rho_p^T(p_{ref}, T)} \frac{\partial \rho_p^p}{\partial T}, \quad p = o, g, w \tag{2.28}$$

$$\frac{\partial \mu_p}{\partial p} = \frac{\mu_p^p(p)}{\mu_p^T(p_{ref}, T)} \frac{\partial \mu_p^p}{\partial T}, \quad p = o, g, w \tag{2.29}$$

$$\frac{\partial U_p}{\partial p} = 0, \quad p = o, g, w \tag{2.30}$$

$$\frac{\partial U_R}{\partial p} = 0 \tag{2.31}$$

$$\frac{\partial H_p}{\partial p} = \frac{\rho_p - P \dfrac{\partial \rho_p}{\partial p}}{\rho_p^2}, \quad p = o, g, w \tag{2.32}$$

$$\frac{\partial x_{cp}}{\partial p} = \begin{cases} -\dfrac{\rho_o^{sc} \rho_g^{sc}}{(\rho_o^{sc} + R_{so}\rho_g^{sc})^2} \dfrac{\partial R_{so}}{\partial p}, & p = o, \quad c = o \\ \dfrac{\rho_o^{sc} \rho_g^{sc}}{(\rho_o^{sc} + R_{so}\rho_g^{sc})^2} \dfrac{\partial R_{so}}{\partial p}, & p = o, \quad c = g \\ 0, & \text{otherwise} \end{cases} \tag{2.33}$$

$$\tag{2.34}$$

$$\frac{\partial \Gamma_p}{\partial p} = -\Gamma \frac{k_{rp}}{\mu_p^2} \frac{\partial \mu_p}{\partial p} \quad p = o, g, w \tag{2.35}$$

$$\frac{\partial \Delta \Phi_p}{\partial p} = \begin{cases} \delta_{p^a}^p - \delta_{p^b}^p - \dfrac{\partial \overline{\rho_o}}{\partial p} g(D^a - D^b), & p = o \\ \delta_{p^a}^p - \delta_{p^b}^p - \dfrac{\partial \overline{\rho_w}}{\partial p} g(D^a - D^b), & p = w \\ \delta_{p^a}^p - \delta_{p^b}^p - \dfrac{\partial \overline{\rho_g}}{\partial p}, & p = g \end{cases} \tag{2.36}$$

$$\frac{\partial Q_p}{\partial p} = -\Gamma^w \frac{k_{rp}}{\mu_p (\log(r_0/r_w) + s)} \left( \frac{p - p_{BH}}{\mu_p} \frac{\partial \mu_p}{\partial p} + 1 \right), \quad p = o, g, w \tag{2.37}$$

$$\tag{2.38}$$

Then we define the saturation derivatives

$$\frac{\partial S_p}{\partial S_{p'}} = \begin{cases} 1, & \text{p = p'} \\ -1, & \text{p = g} \\ 0, & \text{otherwise} \end{cases} \tag{2.39}$$

$$\frac{\partial k_{rp}}{\partial S_{p'}} = \text{see paragraph on relative permeability}, p = o, g, w \tag{2.40}$$

$$\frac{\partial \Gamma_p}{\partial S_{p'}} = \Gamma \frac{\partial k_{rp}}{\partial S_{p'}} \frac{1}{\mu_p}, \quad p = o, g, w \tag{2.41}$$

$$\frac{\partial \Delta \Phi_p}{\partial S_{p'}} = \begin{cases} -\dfrac{\partial P_{cgo}^a}{\partial S_{p'}} + \dfrac{\partial P_{cgo}^b}{\partial S_{p'}}, & p = o \\[2ex] -\dfrac{\partial P_{cgo}^a}{\partial S_{p'}} - \dfrac{\partial P_{cwo}^a}{\partial S_{p'}} + \dfrac{\partial P_{cgo}^b}{\partial S_{p'}} + \dfrac{\partial P_{cwo}^b}{\partial S_{p'}}, & p = w \\[2ex] 0, & p = g \end{cases} \tag{2.42}$$

$$\frac{\partial Q_p}{\partial S_{p'}} = -\Gamma^w \frac{1}{\mu_p \left( \log(r_0/r_w) + s \right)} (p - p_{BH}) \frac{\partial k_{rp}}{\partial S_{p'}}, \quad p = o, g, w \tag{2.43}$$

And finally the temperature derivatives

$$\frac{\partial \rho_p}{\partial T} = \frac{\rho_p(p)}{\rho_p(p_{\text{ref}})} \frac{\partial \rho_p^T(T)}{\partial T} \tag{2.44}$$

$$\frac{\partial \mu_p}{\partial T} = \frac{\mu_p(p)}{\mu_p(p_{\text{ref}})} \frac{\partial \mu_p^T(T)}{\partial T} \tag{2.45}$$

$$\frac{\partial U_p}{\partial T} = (T - T_{ref}) \frac{\partial C_p}{\partial T} + C_p, \quad p = o, g, w \tag{2.46}$$

$$\frac{\partial U_R}{\partial T} = c_{pR} + b(T - T_r ef) \tag{2.47}$$

$$\frac{\partial H_p}{\partial T} = c_{pp} - \frac{P}{\rho_p^2} \frac{\partial \rho_p}{\partial T}, \quad p = o, g, w \tag{2.48}$$

$$\frac{\partial x_{cp}}{\partial T} = 0, \quad c = o, g, w, \quad p = o, g, w \tag{2.49}$$

$$\frac{\partial k_{rp}}{\partial T} = \text{see paragraph on relative permeability}, \quad p = o, g, w \tag{2.50}$$

$$\frac{\partial \Gamma_p}{\partial T} = \Gamma \left( \frac{\partial k_{rp}}{\partial T} \frac{1}{\mu_p} - \frac{k_{rp}}{\mu_p^2} \frac{\partial \mu_p}{\partial T} \right), \quad p = o, g, w \tag{2.51}$$

$$\frac{\partial \Delta \Phi_p}{\partial T} = \frac{\partial \overline{\rho_p}}{\partial T} g(D^a - D^b), \quad p = o, g, w \tag{2.52}$$

$$\frac{\partial Q_p}{\partial T} = -\Gamma^w \frac{1}{\mu_p \left( \log(r_0/r_w) + s \right)} (p - p_{BH}) \left( \frac{\partial k_{rp}}{\partial T} - \frac{k_{rp}}{\mu_p} \frac{\partial \mu_p}{\partial T} \right), \quad p = o, g, w \tag{2.53}$$

$$\tag{2.54}$$

# 3   Compositional model formulation

To find the solution of the compositional problem, we need to solve a similar system as the black-oil system of non-linear equations $F(X) = 0$. But in this case the vector of unknown variables is $X = \{p, T, S_w, S_o, \mathbf{x}, \mathbf{y}\}$ and equations are taken from (1.4)-(1.5). Again we represent the gas saturation $S_g$ as a function of the two other saturations

$$S_g(S_o, S_w) \quad = \quad 1 - S_o - S_w \tag{3.1}$$

We use Newton method to linearize the system of equations

$$J\delta X = -F \tag{3.2}$$

## 3.1   GPRS compositional model

In this section, we use the compositional model based on GPRS assumptions (see 1.3). To obtain the Jacobian, we need to completely derive our system:

$$
\begin{aligned}
\frac{\partial F_c}{\partial p} \quad = \quad & V\Big[\frac{\partial \phi}{\partial p}\sum_p S_p \rho_p x_{cp} + \phi \sum_p S_p \frac{\partial \rho_p}{\partial p}x_{cp}\Big] \\
& - \tau \sum_l \sum_p x_{cp}^l \Big(\frac{\partial \rho_p^l}{\partial p}\Gamma_p^l \Delta\Phi_p^l + \rho_p^l \frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + \rho_p^l \Gamma_p^l \frac{\partial \Delta\Phi_p^l}{\partial p}\Big) \\
& + \tau \sum_p x_{cp}\Big(\frac{\partial \rho_p}{\partial p}Q_p + \rho_p \frac{\partial Q_p}{\partial p}\Big), \quad c = 1,\dots,n_c
\end{aligned}
\tag{3.3}
$$

Similarly, we can calculate the pressure derivatives for the energy equation

$$
\begin{aligned}
\frac{\partial F_e}{\partial p} \quad = \quad & V\Big[\frac{\partial \phi}{\partial p}\Big(\sum_p S_p \rho_p U_p - U_R\Big) + \phi \sum_p\Big(S_p \frac{\partial \rho_p}{\partial p}U_p + S_p \rho_p \frac{\partial U_p}{\partial p}\Big) + (1-\phi)\frac{\partial U_R}{\partial p}\Big] \\
& - \tau \sum_l \sum_p\Big(\frac{\partial H_p^l}{\partial p}\rho_p^l\Gamma_p^l\Delta\Phi_p^l + H_p^l\frac{\partial \rho_p^l}{\partial p}\Gamma_p^l\Delta\Phi_p^l + H_p^l\rho_p^l\frac{\partial \Gamma_p^l}{\partial p}\Delta\Phi_p^l + H_p^l\rho_p^l\Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial p} + \frac{\partial \Gamma_c^l}{\partial p}\Delta T^l\Big) \\
& + \tau \sum_p\Big(\frac{\partial \rho_p}{\partial p}H_p Q_p + \rho_p \frac{\partial H_p}{\partial p}Q_p + \rho_p H_p\frac{\partial Q_p}{\partial p}\Big)
\end{aligned}
\tag{3.4}
$$

Then we calculate the saturation $S_{p'}$ derivatives

$$
\begin{aligned}
\frac{\partial F_c}{\partial S_{p'}} \quad = \quad & V\Big[\phi \sum_p x_{cp}\frac{\partial S_p}{\partial S_{p'}}\rho_p\Big] - \tau \sum_l \sum_p x_{cp}^l\rho_p^l\Big(\frac{\partial \Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l + \Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial S_{p'}}\Big) \\
& + \tau \sum_p x_{cp}\rho_p\frac{\partial Q_p}{\partial S_{p'}}, \quad c = 1,\dots,n_c
\end{aligned}
\tag{3.5}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial S_{p'}} \quad = \quad & V\Big[\phi \sum_p \frac{\partial S_p}{\partial S_{p'}}\rho_p U_p\Big] - \tau \sum_l \sum_p\Big[H_p^l\rho_p^l\Big(\frac{\partial \Gamma_p^l}{\partial S_{p'}}\Delta\Phi_p^l + \Gamma_p^l\frac{\partial \Delta\Phi_p^l}{\partial S_{p'}}\Big) + \frac{\partial \Gamma_c^l}{\partial S_{p'}}\Delta T^l\Big] \\
& + \tau \sum_p \rho_p H_p\frac{\partial Q_p}{\partial S_{p'}}
\end{aligned}
\tag{3.6}
$$

For the compositional system, we also calculate both oil $x_c$ and gas $y_c$ fractions derivatives. However we only present here the oil fractions derivatives

$$
\begin{aligned}
\frac{\partial F_c}{\partial x_c} &= V\Big[\phi\sum_p\Big(\frac{\partial x_{c,p}}{\partial x_c}\rho_p+x_{c,p}\frac{\partial\rho_p}{\partial x_c}\Big)S_p\Big] \\
&\quad - \tau\sum_l\Big(\sum_p\frac{\partial x_{cp}^l}{\partial x_c}\rho_p^l\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\frac{\partial\rho_p^l}{\partial x_c}\Gamma_p^l\Delta\Phi_p^l+x_{cp}^l\rho_p^l\Gamma_p^l\frac{\partial\Delta\Phi_p^l}{\partial x_c}\Big) \\
&\quad + \tau\sum_p\Big(\frac{\partial x_{cp}}{\partial x_c}\rho_p+x_{cp}\frac{\partial\rho_p}{\partial x_c}\Big)Q_p, \quad c=1,\ldots,n_c
\end{aligned}
\tag{3.7}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial x_c} &= V\Big[\phi\sum_p\Big(\frac{\partial\rho_p}{\partial x_c}U_p+\rho_p\frac{\partial U_p}{\partial x_c}\Big)S_p\Big] \\
&\quad - \tau\sum_l\Big(\sum_p\frac{\partial H_p^l}{\partial x_c}\rho_p^l\Gamma_p^l\Delta\Phi_p^l+H_p^l\frac{\partial\rho_p^l}{\partial x_c}\Gamma_p^l\Delta\Phi_p^l+H_p^l\rho_p^l\Gamma_p^l\frac{\partial\Delta\Phi_p^l}{\partial x_c}\Big) \\
&\quad + \tau\sum_p\Big(\frac{\partial\rho_p}{\partial x_c}H_p+\rho_p\frac{\partial H_p}{\partial x_c}\Big)Q_p
\end{aligned}
\tag{3.8}
$$

Finally we need the temperature $T$ derivatives

$$
\begin{aligned}
\frac{\partial F_c}{\partial T} &= V\Big[\phi\sum_p S_p\frac{\partial\rho_p}{\partial T}x_{cp}\Big]-\tau\sum_l\sum_p x_{cp}^l\Big(\frac{\partial\rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l+\rho_p^l\frac{\partial\Gamma_p^l}{\partial T}\Delta\Phi_p^l\Big) \\
&\quad + \tau\sum_p x_{cp}\Big(\frac{\partial\rho_p}{\partial T}Q_p+\rho_p\frac{\partial Q_p}{\partial T}\Big), \quad c=1,\ldots,n_c
\end{aligned}
\tag{3.9}
$$

$$
\begin{aligned}
\frac{\partial F_e}{\partial T} &= V\Big[\phi\sum_p\Big(S_p\frac{\partial\rho_p}{\partial T}U_p+S_p\rho_p\frac{\partial U_p}{\partial T}\Big)+(1-\phi)\frac{\partial U_R}{\partial T}\Big] \\
&\quad - \tau\sum_l\sum_p\Big(\frac{\partial H_p^l}{\partial T}\rho_p^l\Gamma_p^l\Delta\Phi_p^l+H_p^l\frac{\partial\rho_p^l}{\partial T}\Gamma_p^l\Delta\Phi_p^l+H_p^l\rho_p^l\frac{\partial\Gamma_p^l}{\partial T}\Delta\Phi_p^l+\frac{\partial\Gamma_c^l}{\partial T}\Delta T^l+\Gamma_c^l\frac{\partial\Delta T^l}{\partial T}\Big) \\
&\quad + \tau\sum_p\Big(\frac{\partial\rho_p}{\partial T}H_pQ_p+\rho_p\frac{\partial H_p}{\partial T}Q_p+\rho_pH_p\frac{\partial Q_p}{\partial T}\Big)
\end{aligned}
\tag{3.10}
$$

## 3.2 GPRS correlations for compositional model

### 3.2.1 Water phase properties

We take the same description as the one described in the Black-Oil section. Note that an alternative for the water properties is developed in the Appendix section.

### 3.2.2 Hydrocarbon properties

- Density
  The molar density $\rho_m$ (lbmol/cuft)is defined as the inverse of the molar volume $V_m$:

$$
\rho_m=\frac{1}{V_m}
$$

and $V_m$ is obtained using the non ideal gas equation:

$$V_m = \frac{ZRT}{P} - c$$

where

Z    is the compressibility factor (dimensionless)
R    is the ideal gas constant (=10.73 psi.cuft/lbmol.°R)
T    is the temperature in ° R
P    is the pressure in psi
c    is a volume translation.

The density is obtained by multiplying the molar density by the phase molar mass:

$\rho = \rho_m M$, for a given phase.

The derivatives of the density are given by:

$$\frac{\partial \rho}{\partial x_i} = -\frac{\rho}{Z}\frac{\partial Z}{\partial x_i}, \text{ for } i = 1, \dots, n_h$$
$$\frac{\partial \rho}{\partial P} = \frac{\rho}{P} - \frac{\rho}{Z}\frac{\partial Z}{\partial P}$$
$$\frac{\partial \rho}{\partial T} = -\rho \left( \frac{1}{Z}\frac{\partial Z}{\partial T} + \frac{1}{T} \right).$$

- Viscosity
  We use the description given in [10]. Viscosities are expressed in (cP). The calculation procedure is as follows (the first two steps are common to both gas and liquid viscosity calculations):

  – get the low-pressure pure-component gas viscosities at the temperature of interest using:

  $$\mu_j^* \zeta_j = 34 \times 10^{-5} T_{rj}^{0.94}, (T_{rj} < 1.5),$$
  $$\mu_j^* \zeta_j = 17.78 \times 10^{-5} (4.58 T_{rj} - 1.67)^{5/8}, (T_{rj} > 1.5),$$

  – get the low-pressure mixture gas viscosity at the temperature of interest using:

  $$\mu^* = \frac{\displaystyle\sum_{j=1}^{n_c} (x_j \mu_j^* \sqrt{M_j})}{\displaystyle\sum_{j=1}^{n_c} (x_j \sqrt{M_j})}$$

  – get the viscosity of the liquid mixture using:

  $$\mu = \mu^* + \frac{1}{\zeta} \left( (A + B\rho_r + C\rho_r^2 - D\rho_r^3 + E\rho_r^4)^4 - 1 \times 10^{-4} \right)$$

where

$\mu_j^*$        is the viscosity of component $j$ as a gas at low pressure (in cP)

$T_{rj} = \dfrac{T}{T_{cj}}$        is the reduced temperature of component $j$

$P_{cj}$        is the critical pressure of component $j$ (in atm)

$T_{cj}$        is the critical pressure of component $j$ (in K)

$M_j$        is the molar weight of component $j$ (g/mol)

$x_j$        is the mole fraction of component $j$

$\zeta_j = \dfrac{T_{cj}^{1/6}}{M_j^{1/2} P_{cj}^{2/3}}$        is the viscosity parameter of component $j$

$\zeta = \dfrac{\left[ \sum\limits_{j=1}^{n_c} (x_j T_{cj}) \right]^{1/6}}{\left[ \sum\limits_{j=1}^{n_c} (x_j M_j) \right]^{1/2} \left[ \sum\limits_{j=1}^{n_c} (x_j P_{cj}) \right]^{2/3}}$        is the viscosity parameter of a mixture

and

| $A$ | $=$ | 0.1023 | $B$ | $=$ | 0.023364 | $C$ | $=$ | 0.058533 |
|---|---|---|---|---|---|---|---|---|
| $D$ | $=$ | 0.40758 | $E$ | $=$ | 0.0093324. | | | |

$\frac{\partial \mu}{\partial p}$ and $\frac{\partial \mu}{\partial T}$ are currently set to zero in GPRS.

- Enthalpy
  We take the description given by [12].
  The system enthalpy $H$ (in Btu/lb) of a fluid which follows a cubic equation of state (Peng-Robinson in our case) is given by the sum of the enthalpy at the ideal gas state $H^*$ and the excess enthalpy $H_E$ :

$H = H^* + \gamma H_E$ with $\gamma = 0$ or 1.Currently $\gamma$ is set equal to zero.

where

$$H^* = \sum_{i=1}^{n_c} x_i H_i^*$$

$$H_i^* = H_A + H_B T + H_C T^2 + H_D T^3 + H_E T^4 + H_F T^5$$

$$H_E = P V_m - RT + \frac{1}{\delta_2 - \delta_1} \left( T \frac{\partial a}{\partial T} - a \right) \ln \left( \frac{V_m + \delta_2 b}{V_m + \delta_1 b} \right)$$

$$\delta_1 = 1 - \frac{\sqrt{u^2 - 4w}}{2}$$

$$\delta_2 = -1/\delta_1.$$

$H_A, \ldots, H_F$ are user specified parameters given by [14], $T$ unit is R.

Currently $H^* = H_i^* = H_A + H_B T + H_C T^2$

The derivatives are given by:

$$\frac{\partial H}{\partial x_i} = \frac{\partial H^*}{\partial x_i} + \gamma \frac{\partial H_E}{\partial x_i}$$

with

$$\frac{\partial H^*}{\partial x_i} = H_i^*$$

$$\frac{\partial H_E}{\partial x_i} = RT\frac{\partial Z}{\partial x_i} - P\frac{\partial c}{\partial x_i} + \frac{1}{\delta_2 - \delta_1}\ln\left(\frac{V_m + \delta_2 b}{V_m + \delta_1 b}\right)\left(T\frac{\partial^2 a}{\partial T^2} - \frac{\partial a}{\partial x_i}\right)$$
$$+ \frac{1}{(V_m + \delta_2 b)(V_m + \delta_1 b)}\left(T\frac{\partial a}{\partial T} - a\right)\left(V_m\frac{\partial b}{\partial x_i} - b\left(\frac{1}{P}RT\frac{\partial Z}{\partial x_i} - \frac{\partial c}{\partial x_i}\right)\right)$$

$$\frac{\partial H}{\partial P} = \gamma \frac{\partial H_E}{\partial P}$$

with

$$\frac{\partial H_E}{\partial P} = V_m + \left(\frac{\partial Z}{\partial P} - \frac{Z}{P}\right)RT\left(1 - \frac{b}{P(V_m + \delta_2 b)(V_m + \delta_1 b)}\left(T\frac{\partial a}{\partial T} - a\right)\right)$$

$$\frac{\partial H}{\partial T} = \frac{\partial H^*}{\partial T} + \gamma \frac{\partial H_E}{\partial T}$$

with

$$\frac{\partial H^*}{\partial T} = \sum_{i=1}^{n_c} x_i(H_B + 2H_C T + 3H_D T^2 + 4H_E T^3 + 5H_F T^4)$$

$$\frac{\partial H_E}{\partial T} = R\left(T\frac{\partial Z}{\partial T} + Z - 1\right)$$
$$+ \frac{1}{\delta_2 - \delta_1}\left(T\frac{\partial^2 a}{\partial T^2}\ln\left(\frac{V_m + \delta_2 b}{V_m + \delta_1 b}\right) - \frac{(\delta_2 - \delta_1)Rb}{P(V_m + \delta_2 b)(V_m + \delta_1 b)}\left(T\frac{\partial Z}{\partial T} + Z\right)\left(T\frac{\partial a}{\partial T} - a\right)\right).$$

### 3.2.3 Fugacity

The fugacity of component $i$ is given by:

$$f_i = pX_i\exp^{\Phi_i}$$

$$\Phi_i = \frac{b_i}{b}(Z-1) - \ln(Z-B) + \frac{A}{B\sqrt{u^2-4w}}\left(\frac{b_i}{b} - \frac{1}{a}\frac{\partial a}{\partial X_i}\right)\ln\left[\frac{2Z + B(u + \sqrt{u^2-4w})}{2Z + B(u - \sqrt{u^2-4w})}\right]$$

$$\frac{\partial f_i}{\partial T} = f_i\frac{\partial \Phi_i}{\partial T}$$

$$\frac{\partial \Phi_i}{\partial T} = \frac{b_i}{b}\frac{\partial Z}{\partial T} - \frac{\frac{\partial Z}{\partial T} - \frac{\partial B}{\partial T}}{Z-B} + \left(\frac{b_i}{b} - \frac{1}{a}\frac{\partial a}{\partial X_i}\right)\frac{1}{\sqrt{u^2-4w}}$$

$$\left[\left(\frac{1}{B}\frac{\partial A}{\partial T} - \frac{A}{B^2}\frac{\partial B}{\partial T}\right)\ln\left(\frac{2Z + B(u + \sqrt{u^2-4w})}{2Z + B(u - \sqrt{u^2-4w})}\right) + \frac{A}{B}\left(\frac{2\frac{\partial Z}{\partial T} + \frac{\partial B}{\partial T}(u + \sqrt{u^2-4w})}{2Z + B(u + \sqrt{u^2-4w})} - \frac{2\frac{\partial Z}{\partial T} + \frac{\partial B}{\partial T}(u - \sqrt{u^2-4w})}{2Z + B(u - \sqrt{u^2-4w})}\right)\right]$$

$$+ \frac{1}{a}\left(\frac{\partial^2 a}{\partial T \partial X_i} - \frac{1}{a}\frac{\partial a}{\partial T}\frac{\partial a}{\partial X_i}\right)\frac{A}{B\sqrt{u^2-4w}}\ln\left[\frac{2Z + B(u + \sqrt{u^2-4w})}{2Z + B(u - \sqrt{u^2-4w})}\right]$$

$A, B, Z, a, b$ are defined in [2].

### 3.2.4  Z factor

The compressibility factor is given by:

$$Z^3 + sZ^2 + qZ + r = 0$$
and

$$\frac{\partial Z}{\partial T} = -\frac{\frac{\partial s}{\partial T}Z^2 + \frac{\partial q}{\partial T}Z + \frac{\partial r}{\partial T}}{3Z^2 + 2sZ + q}$$
where

$$s = (u-1)B - 1$$
$$q = A + (w-u)B^2 - uB$$
$$r = -AB - wB^2 - wB^3$$
$u, v, w$ are defined in [2].

# 4  Steam model formulation

## 4.1  Steam property

If we consider the steam injection case, which means there is water component in gas phase. We can calculate the density, viscosity and molar fraction of steam in gas phase.

### 4.1.1  Steam density

The steam density is calculated from the real gas law:

$$\rho_{\text{steam}} = \rho_{\text{steam},b}\frac{T_b}{T}$$

where $T_b$ is the boiling point temperature and is the function of pressure, and $\rho_{\text{steam},b}$ is the density at the boiling point. The saturated water vapor density is given by

$$\rho_{\text{steam},b} = \exp[a_0 + a_1 T_b + a_2 T_b^2 + a_3 T_b^3 + a_4 T_b^4 + a_5 T_b^5]$$

where, $\rho_{\text{steam},b}$ is in lbmol/cuft, $T_b$ is the boiling point temperature in R. The correlation of $T_b$ is

$$T_b = b_0 + b_1 \ln p + b_2 (\ln p)^2 + b_3 (\ln p)^3 + b_4 (\ln p)^4$$

Herein

| | | | | | |
|---|---|---|---|---|---|
| $a_0$ = -96.4809 | | $a_1$ = 0.463301 | | $a_2$ = $-9.90153 \times 10^{-4}$ | |
| $a_3$ = $1.12766 \times 10^{-6}$ | | $a_4$ = -6.60862 $\times 10^{-10}$ | | $a_5$ = $1.57286 \times 10^{-13}$. | |

and

| | | | |
|---|---|---|---|
| $b_0$ = 561.435 | $b_1$ = 33.8866 | $b_2$ = 2.18893 | |
| $b_3$ = 0.0808998 | $b_4$ = 0.0342030. | | |

The derivatives are given by:

$$\frac{\partial \rho_{\text{steam}}}{\partial p} = \frac{1}{T}\frac{\partial T_b}{\partial p}\rho_{\text{steam},b} + \frac{1}{T}\frac{\partial T_b}{\partial p}\rho_{\text{steam},b}(a_1 T_b + 2a_2 T_b^2 + 3a_3 T_b^3 + 4a_4 T_b^4 + 5a_5 T_b^5)$$

$$\frac{\partial \rho_{\text{steam}}}{\partial T} = -\frac{\rho_{\text{steam}}}{T}$$
$$\frac{\partial T_b}{\partial p} = \frac{1}{p}(b_1 + 2b_2(\ln p) + 3b_3(\ln p)^2 + 4b_4(\ln p)^3)$$

### 4.1.2 Steam viscosity

The steam viscosity is given by:

$$\mu_{\text{steam}} = A_g + B_g T + C_g p^{D_g} \tag{4.1}$$

where the unit of temperature $T$ is R, the unit of pressure $p$ is Psi
and $A_g = -8.9784 \times 10^{-3}$, $B_g = 2.8309 \times 10^{-5}$, $C_g = 1.11 \times 10^{-11}$, $D_g = 2.5077$.

The derivatives are:

$$\frac{\partial \mu_{\text{steam}}}{\partial p} = C_g D_g p^{D_g-1}$$
$$\frac{\partial \mu_{\text{steam}}}{\partial T} = B_g$$

### 4.1.3 Steam enthalpy

The steam specific enthalpy can be calculated as

$$H_s = c_0 + c_1 T + c_2 T^2 + c_3 T^3 + c_4 T^4 + c_5 T^5 + c_6 T^6 \tag{4.2}$$

Herein

| | | | | | | |
|---|---|---|---|---|---|---|
| $c_0$ | = | -9469.85 | $c_1$ | = | 87.2545 | $c_2$ | = | -0.299668 |
| $c_3$ | = | $5.4361 \times 10^{-4}$ | $c_4$ | = | $-5.46484 \times 10^{-7}$ | $c_5$ | = | $2.88759 \times 10^{-10}$ |
| $c_6$ | = | $-6.28068 \times 10^{-14}$. | | | | | |

The derivatives are

$$\frac{\partial H_s}{\partial p} = 0$$
$$\frac{\partial H_s}{\partial T} = c_1 + 2c_2 T + 3c_3 T^2 + 4c_4 T^3 + 5c_5 T^4 + 6c_6 T^5$$

### 4.1.4 Steam molar concentration

When steam exists, the molar concentration of water in gas phase will be

$$y_s = x_{w,g} = \frac{p_{sat}(T)}{p} \tag{4.3}$$

Where $y_s$ is the molar fraction of steam in gas phase. And $p_{sat}(T)$ is the saturation pressure of steam, which can be got from steam table or using the correlation below,

$$p_{sat}(T) = (d_0 + d_1 T + d_2 T^2 + d_3 T^3 + d_4 T^4 + d_5 T^5)^2 \tag{4.4}$$

Herein

$$
\begin{array}{llll}
d_0 & = & \text{-66.9421} & \quad d_1 = 0.485086 \quad d_2 = \text{-1.33944} \times 10^{-3} \\
d_3 & = & 1.71599 \times 10^{-6} & \quad d_4 = \text{-9.93039} \times 10^{-10} \quad d_5 = 2.29394 \times 10^{-13}.
\end{array}
$$

The derivative of molar fraction on pressure is

$$\frac{\partial y_s}{\partial p} = -\frac{p_{sat}(T)}{p^2}$$

The derivative of molar fraction on temperature is

$$\frac{\partial y_s}{\partial T} = \frac{\partial p_{sat}(T)}{\partial T} \frac{1}{p}$$

Where

$$\frac{\partial p_{sat}}{\partial T} = 2(d_0 + d_1 T + d_2 T^2 + d_3 T^3 + d_4 T^4 + d_5 T^5)(d_1 + 2d_2 T + 3d_3 T^2 + 4d_4 T^3 + 5d_5 T^4) \tag{4.5}$$

## 4.2 Mixing rules for gas phase

### 4.2.1 Update of hydrocarbon components molar concentration in Gas Phase

The hydrocarbon components in gas phase can be updated as

$$x_{c,g} = y_c(1 - y_s). \tag{4.6}$$

Here $y_c$ denotes the hydrocarbon molar fraction in vapor phase, $x_{c,g}$ denotes the components molar fractions in gas phase.

The derivative of molar fractions on pressure is

$$\frac{\partial x_{c,g}}{\partial p} = \frac{\partial y_c}{\partial p}(1 - y_s) - y_c \frac{\partial y_s}{\partial p}$$

The derivative of molar fractions on temperature is

$$\frac{\partial x_{c,g}}{\partial T} = \frac{\partial y_c}{\partial T}(1 - y_s) - y_c \frac{\partial y_s}{\partial T}$$

### 4.2.2 Gas phase density

The gas phase molar density is calculated as

$$\rho_g = \frac{p}{zRT} \tag{4.7}$$

Where $z$ factor can be calculated through the equation below

$$z = y_s z_s + (1 - y_s) z_v \tag{4.8}$$

Herein $z_s$ can be calculated from the density of steam

$$z_s = \frac{1}{\rho_s RT}$$

The derivative on pressure is

$$\frac{\partial \rho_g}{\partial p} = \frac{1}{zRT} - \frac{p}{z^2 RT}\frac{\partial z}{\partial p} = \frac{1}{zRT} - \frac{p}{z^2 RT}\left(\frac{\partial y_s}{\partial p}z_s + \frac{\partial z_s}{\partial p}y_s - \frac{\partial y_s}{\partial p}z_v + (1-y_s)\frac{\partial z_v}{\partial p}\right)$$

The derivative on temperature is

$$\frac{\partial \rho_g}{\partial T} = -\frac{p}{zRT^2} - \frac{p}{z^2 RT}\left(\frac{\partial y_s}{\partial T}z_s + \frac{\partial z_s}{\partial T}y_s - \frac{\partial y_s}{\partial T}z_v + (1-y_s)\frac{\partial z_v}{\partial T}\right)$$

### 4.2.3 Gas phase enthalpy

The mixed gas internal energy $H_g$ is

$$H_g = y_s H_s + (1-y_s)H_v \tag{4.9}$$

$H_s$ is the molar enthalpy of steam, and $H_v$ is the total molar enthalpy of hydrocarbon in gas phase.
The derivative on pressure is

$$\frac{\partial H_g}{\partial p} = \frac{\partial y_s}{\partial p}H_s + \frac{\partial H_s}{\partial p}y_s - \frac{\partial y_s}{\partial p}H_v + (1-y_s)\frac{\partial H_v}{\partial p}$$

The derivative on temperature is

$$\frac{\partial H_g}{\partial T} = \frac{\partial y_s}{\partial T}H_s + \frac{\partial H_s}{\partial T}y_s - \frac{\partial y_s}{\partial T}H_v + (1-y_s)\frac{\partial H_v}{\partial T}$$

### 4.2.4 Gas phase viscosity

The mixing rule of gas phase viscosity is same as that of density.

$$\mu_g = y_s \mu_s + (1-y_s)\mu_v \tag{4.10}$$

$\mu_s$ is the viscosity of steam, and $\mu_v$ is the viscosity of hydrocarbon in gas phase.
The derivative on pressure is

$$\frac{\partial \mu_g}{\partial p} = \frac{\partial y_s}{\partial p}\mu_s + \frac{\partial \mu_s}{\partial p}y_s - \frac{\partial y_s}{\partial p}\mu_v + (1-y_s)\frac{\partial \mu_v}{\partial p}$$

The derivative on temperature is

$$\frac{\partial \mu_g}{\partial T} = \frac{\partial y_s}{\partial T}\mu_s + \frac{\partial \mu_s}{\partial T}y_s - \frac{\partial y_s}{\partial T}\mu_v + (1-y_s)\frac{\partial \mu_v}{\partial T}$$

# 5 Phase split calculation

This section provides a short description of the conventional method for solving isothermal compositional phase split calculation as well as similar calculation with the presence of steam.

## 5.1 Thermodynamic system of equation

For a general multi-phase, $n_p$, multi-component, $n_c$, system in thermodynamic equilibrium, we need to solve the following equations:

$$f_{i,j}(p,T,x_{i,j}) - f_{i,k}(p,T,x_{i,k}) = 0, \quad \forall j \neq k \in \{1,\ldots,n_p\}, \quad i \in [1,\ldots n_c], \tag{5.1}$$

$$Z_i - \sum_{j=1}^{n_p} v_j x_{i,j} = 0, \quad i \in [1,\ldots n_c], \tag{5.2}$$

$$\sum_{j=1}^{n_p} v_j - 1 = 0, \tag{5.3}$$

$$\sum_{i=1}^{n_c}(x_{i,j} - x_{i,k}) = 0, \quad \forall j \neq k \in \{1,\ldots,n_p\}. \tag{5.4}$$

Here $p, T$, and $Z_i$ denote pressure, temperature and overall mole fractions of component $i$, respectively; $x_{i,j}$ and $v_p$ represent phase mole fractions; $f_{i,j}(p,T,x_{i,j})$ is the fugacity of component $i$ in phase $j$. We assume that $p, T$, and $Z_i$ are known variables and that $f_{i,j}$ is a known non-linear function. We need to find $x_{i,j}$ and $v_p$.

In practice, we usually assume that the number of phases, $n_p$, is three. A common assumption is that hydrocarbons do not appear in the water phase and that the water component exists in the water phase only. Using these assumptions we can simplify (5.1)-(5.4) to obtain the following system:

$$f_{i,1}(p,T,y_i) - f_{i,2}(p,T,x_i) = 0, \quad i \in [1,\ldots n_h], \tag{5.5}$$
$$z_k - Vy_i - Lx_i = 0, \quad i \in [1,\ldots n_h], \tag{5.6}$$
$$L + V - 1 = 0, \tag{5.7}$$
$$\sum_{i=1}^{n_h}(x_i - y_i) = 0. \tag{5.8}$$

Where $n_h = n_c - 1$ is the the number of hydrocarbon components, subscripts $1, 2$ and $3$ correspond to the gas, oil and water phases respectively. We also present the new notifications

$$V = v_1/(1-v_3), \quad L = v_2/(1-v_3), \quad z_i = Z_i/(1-v_3). \tag{5.9}$$

Since hydrocarbon components can exist in the two hydrocarbon phases only, the mole fractions $x_{i,j}$ become $y_i = x_{i,1}$ and $x_i = x_{i,2}$.

For compositional simulation, we usually need to solve the following problem to describe the phase behavior at equilibrium.

- Phase stability test - for the current $p, T$ and $z_i$, find the phase state (liquid, vapor or two-phase) of this composition. This test is needed for any cell whose status at the previous Newton iteration was single-phase.

- Flash calculation - if the phase stability test indicates that the phase state of the cell changed from single to two phases, we need to solve the system (5.5) - (5.8) in order to obtain the $x_i$, $y_i$ and $V$ ($L$). Note that the K values from the stability analysis can be used as an initial guess.

When steam (water component in vapor phase) is present, we need to change the system (5.5) - (5.8). Following system of equations presented complete description of flash problem with the presence of steam

$$f_{i,j}(p,T,x_{i,j}) - f_{i,k}(p,T,x_{i,k}) = 0, \quad \forall j \neq k \in \{1,\ldots,n_p\}, \quad i \in [1,\ldots n_c], \tag{5.10}$$

$$f_{w,1}(p,T,x_{w,1}) - f_{w,3}(p,T) = 0, \tag{5.11}$$

$$Z_i - \sum_{j=1}^{n_p} v_j x_{i,j} = 0, \quad i \in [1,\ldots n_c], \tag{5.12}$$

$$Z_w - v_1 x_{w,1} - v_3 x_{w,3} = 0, \tag{5.13}$$

$$\sum_{j=1}^{n_p} v_j - 1 = 0, \tag{5.14}$$

$$\sum_{i=1}^{n_c} (x_{i,j} - x_{i,k}) = 0, \quad \forall j \neq k \in \{1,\ldots,n_p\}. \tag{5.15}$$

Usually $x_{w,1} \equiv y_s(p,T)$ - steam fraction can be explicitly found from (5.11), $x_{w,3} \equiv 1$ as long as no hydrocarbon component is present in the water phase. The system for steam injection can be written in a manner similar to the compositional problem using notifications described in (5.9)

$$f_{i,1}(p,T,y_i) - f_{i,2}(p,T,x_i) = 0, \quad i \in [1,\ldots n_h], \tag{5.16}$$

$$z_k - Vy_i - Lx_i = 0, \quad i \in [1,\ldots n_h], \tag{5.17}$$

$$L + V - 1 = 0, \tag{5.18}$$

$$\sum_{i=1}^{n_h} (x_i - y_i) - y_s(p,T) = 0. \tag{5.19}$$

Notice, that for this model constraints for molar fractions $z_i$ and vapor fraction $y_i$ will transform to

$$\sum_{i=1}^{n_h} z_i = 1 - Vy_s \tag{5.20}$$

$$\sum_{i=1}^{n_h} y_i = 1 - y_s. \tag{5.21}$$

Solution of initial problem (5.10) - (5.15) could be transformed to solution of the system (5.16) - (5.19) with additional non-linear constraint (5.21).

## 5.2 Flash calculation

Here we present the standard flash calculation approach using a successive substitution iteration (SSI) algorithm.

1. Calculate an initial guess for $K_i = y_i/x_i$:

$$p_{si} = e^{5.373(1+\omega_i)(1-T_{ci}/T)} p_{ci}, \quad K_i = p_{si}/p, \tag{5.22}$$

   where $p_{ci}$ and $T_{ci}$ denote the critical pressure and temperature for component $i$, and $\omega_i$ is the acentric factor.

2. Calculate $V$ from

$$F(V) = \sum_{i=1}^{N} \frac{z_i(1-K_i)}{V(K_i-1)+1} = 0 \tag{5.23}$$

   Notice that the function $F(V)$ is monotonically decreasing on every interval in its domain.

3. Calculate vapor concentrations

$$y_i = \frac{z_i K_i}{V(K_i - 1) + 1} \tag{5.24}$$

4. Calculate parameters $A$ and $B$ for the EOS

$$A = \sum_{j=1}^{N} \sum_{k=1}^{N} y_j y_k A_{jk}, \quad B = \sum_{j=1}^{N} y_j B_j \tag{5.25}$$

where $A_{jk}$ and $B_j$ - derived from user defined parameters

5. Solve a cubic equation of the form

$$Z^3 + E_2 Z^2 + E_1 Z + E_0 = 0, \tag{5.26}$$

where,

$$E_2 = (m_1 + m_2 - 1)B - 1, \tag{5.27}$$
$$E_1 = A - (2(m_1 + m_2) - 1)B^2 - (m_1 + m_2)B,$$
$$E_0 = -\left(AB + m_1 m_2 B^2 (B + 1)\right).$$

Here $m_1$ and $m_2$ are user defined parameters for the specific EOS used. The maximum positive real root is used for the Z-factor of the vapor phase

6. Calculate the fugacity of components in the vapor phase using

$$\begin{aligned} \ln f_{i,V} \;=\;& \ln(y_i p) - \ln(Z - B) \\ &+ \frac{A}{(m_1 - m_2)B} \left( \frac{2}{A} \sum_{j=1}^{N} y_j A_{ij} - \frac{B_i}{B} \right) \ln \frac{Z + m_2 B}{Z + m_1 B} + \frac{B_i}{B}(Z - 1) \end{aligned} \tag{5.28}$$

7. Similar calculations are performed for the liquid phase in order to find $\ln f_{i,L}$

8. if $| f_{i,L}/f_{i,V} - 1 | < \varepsilon$, we assume that the procedure converged. Otherwise $K_i^{(m)} = K_i^{(m-1)} \frac{f_{i,L}}{f_{i,V}}$ and go to step 2.

In the presence of steam, the only difference will be in step 2. This equation will be transformed to

$$F(V) = \sum_{i=1}^{N} \frac{z_i(1 - K_i)}{V(K_i - 1) + 1} - y_s(p, T) = 0 \tag{5.29}$$

Here $y_s(p, T)$ is the mole fraction of steam in the vapor phase.

Another modification - recalculation of the total fraction $z_i$ on each SSI iteration using (5.21).

## 5.3   Stability test

First we need to determine the phase state (single-phase or two-phase) of composition $z_i$. For this purpose, we check the stability of both the liquid and gas phases. The stability criterion expressed in terms of the mole fraction and fugacity coefficient $\Phi_i = f_i/(y_i p)$ can be written as

$$\sum_{i=1}^{N} \left( \ln y_i + \ln \Phi_i(y) - \ln z_i - \ln \Phi_i(z) \right) \geq 0. \tag{5.30}$$

It can be shown that the minimum of the left hand side is a stationary point satisfying

$$\ln y_i + \ln \Phi_i(\mathbf{y}) - \ln z_i - \ln \Phi_i(\mathbf{z}) = \eta,$$

where $\eta$ is independent of $i$. We introduce

$$\ln Y_i = \ln y_i - \eta \Leftrightarrow y_i = Y_i e^{\eta} \tag{5.31}$$

and equation (5.31) can be rewritten as

$$F_i \equiv \ln Y_i + \ln \Phi_i(\mathbf{y}) - \ln z_i - \ln \Phi_i(\mathbf{z}) = 0, \quad i = 1, \dots, N. \tag{5.32}$$

Introducing $K_i = Y_i/z_i$ into equation (5.32)

$$F_i \equiv \ln K_i + \ln \Phi_i(\mathbf{y}) - \ln \Phi_i(\mathbf{x}) = 0, \quad i = 1, \dots, N \tag{5.33}$$

This non-linear system of equations must be solved for the unknowns $\alpha_i = \ln K_i$.

Using the initial estimate for $K_i$ (5.22), we can calculate an initial estimate for $X_i$

$$X_i = z_i/K_i. \tag{5.34}$$

For the liquid-phase check, the initial guess can be found from

$$Y_i = z_i K_i. \tag{5.35}$$

Using (5.28) for both phases, calculate the fugacities $\ln f_{i,V}(z)$ and $\ln f_{i,L}(x)$, substitute into (5.32), and repeat iterations until convergence. If the resulting $\sum_{i=1}^{N} Y_i < 0$ from the trial calculations of (5.31), this phase is stable. If both phases are unstable, we need to perform the flash calculation. For the flash calculation, molar compositions from (5.32) serve as a good initial guess for $x_i$ and $y_i$.

## 5.4   Extension of the GPRS framework to thermal

Modern hydrodynamic simulators used combination of implicit and explicit discretization for base physical variables. Usually for solution of derived system Newton method is used.

Lets present system of non-linear equation that could be effectively solved by hydrodynamic simulator

$$F_i(X) = 0, \quad i = 1, \dots, n, \quad X = \{X_1, \dots X_n\}. \tag{5.36}$$

For solution of this non-linear system we use Newton method. For each Newton iteration we need to solve linear system

$$\frac{\partial F_i}{\partial X_j} \Delta X = -F_i(X). \tag{5.37}$$

Extension for the system (5.36) could be presented as following system

$$X_i = X_i(Y) \quad , \quad i = 1, \ldots, n, \quad Y = \{Y_1, \ldots Y_m\}, m > n, \tag{5.38}$$

$$F_i(X(Y)) = 0 \quad , \quad i = 1, \ldots, n, \tag{5.39}$$

$$G_k(Y) = 0 \quad , \quad k = 1, \ldots, m - n. \tag{5.40}$$

Resulting Jacobian for this system could be written as

$$\frac{\partial F_i}{\partial Y_j} \Delta Y = -F_i(Y), \tag{5.41}$$

$$\frac{\partial G_k}{\partial Y_j} \Delta Y = -G_k(Y).$$

Lets use chain rule for first equation from (5.41). Finally system of equation could be presented as

$$\frac{\partial F_i}{\partial X} \frac{\partial X}{\partial Y_j} \Delta Y = -F_i(X(Y)), \tag{5.42}$$

$$\frac{\partial G_k}{\partial Y_j} \Delta Y = -G_k(Y).$$

Main idea is to use as much as possible from existed solution of (5.36). Following algorithm could be suggested as such method

- Make discretization of (5.36) using existed procedures to obtain (5.37)

- Extend jacobian (5.37) in order to include new variables and derivatives

- Update linear equation using (5.42)

- Solve new linear system and update extended variables $Y$

- Reduce extended variables $Y$ to initial $X$ using (5.38)

# 6  Relative permeability

Relative permeability parameters, measured at full reservoir conditions of pressure and temperature, are essential for reservoir simulations to predict recoverable reserves and to evaluate the economic impact of waterfloods or other enhanced recovery schemes. The concept of relative permeability is very simple, the measurement and interpretation of relative permeability versus saturation curves is not. For example, there is evidence that relative permeability may be a function of many more parameters than fluid saturation. Temperature, flow velocity, saturation history, wettability changes and the mechanical and chemical behaviour of the matrix material may all play roles in changing the functional dependence of the relative permeability on saturation. The best defined of these dependences is the variation of relative permeability with saturation history; it is then often assumed that relative permeabilities are functions of fluid saturation only. Based on a strict wettability argument ($w > o > g$), it is common to assume:

$$k_{rw} = k_{rw}(S_w), \; k_{rg} = k_{rg}(S_g), \; k_{ro} = k_{ro}(S_w, S_g),$$

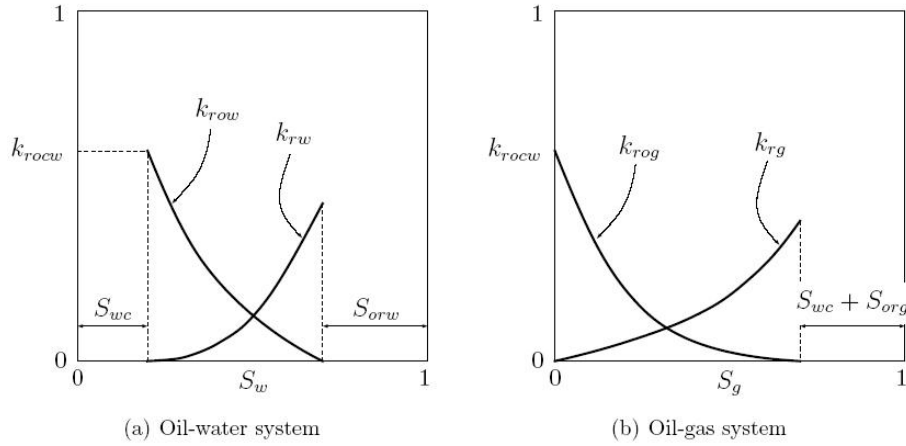where $k_{ro}$ is interpolated from two-phase experiments.

Figure 1: Two-phase relative permeabilities for an oil-water system (left) and an oil-gas system at connate water saturation (right). PE224 material.

## 6.1 Two-phase relative permeability

Water and gas relative permeabilities are obtained from two-phase experiments (see Figure 1).

- $S_p$ – phase $p$, $p = g,o,w$ saturation,

- $S_{wc}$ – connate water saturation,

- $S_{orw}$ – residual oil saturation to water,

- $S_{org}$ – residual oil saturation to gas,

- $k_{rp}$ – phase $p$, $p = g,o,w$ relative permeability,

- $k_{rwc}$ – water relative permeability at residual oil saturation,

- $k_{rgc}$ – gas relative permeability at residual oil saturation and irreducible water saturation,

- $k_{row}$ – oil relative permeability in a water-oil displacement,

- $k_{rog}$ – oil relative permeability in an oil-gas displacement and irreducible water,

- $k_{rocw}$ – oil relative permeability at connate water displacement.

Oil relative permeability is interpolated from these two-phase experiments. There are many interpolation methods available; Stone I, Stone II and Baker are the most common. But whatever the interpolation method, it is essential (and not always recognized) that the two-phase relative permeabilities come from experiments that reproduce a similar saturation path to that of the three-phase case being predicted. In the following paragraph, we are only discussing Baker method.

## 6.2 Three-phase relative permeability

### 6.2.1 Ternary diagram

Ternary diagram are used to represent the relative percentage of three components. These components can be anything. The only requirement is that the three components have to sum to 100 %. Figure 2 is a ternary diagram, where any point represents the relative percentage of three components: GAS, OIL, WATER.
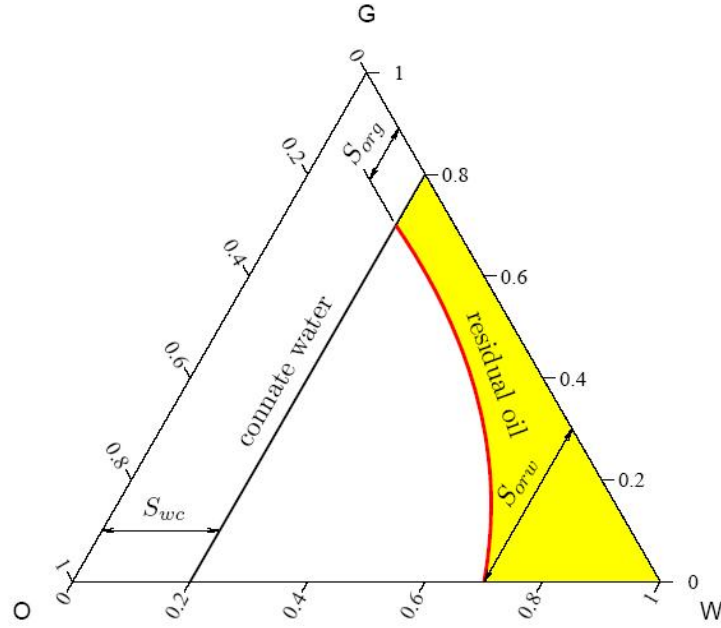
Figure 2: Ternary diagram. PE224 material.

### 6.2.2 Baker model

Baker used a saturation-weighted interpolation between two-phase relative permeability experiments (oil-water imbibition and oil-gas drainage for a water-wet media) to find the value of the three-phase oil relative permeability:

$$k_{ro}(S_w, S_g) = \frac{S_g \overline{k_{rog}} + (S_w - S_{wc}) \overline{k_{row}}}{S_g + (S_w - S_{wc})}$$

Where, the two phase relative permeabilities are evaluated at the same oil saturation:

$\overline{k_{row}} = k_{row}(1 - S_o) = k_{row}(S_g + S_w)$

$\overline{k_{row}} = \overline{k_{row}}(S_g, S_o)$

$\overline{k_{rog}} = k_{rog}(1 - S_o - S_{wc}) = k_{rog}(S_g + S_w - S_{wc})$

$\overline{k_{rog}} = \overline{k_{rog}}(S_g, S_o)$

N.B: Baker model works with actual saturations and actual relative permeabilities.

Keeping in mind that $S_g$ and $S_o$ are primary variables in GPRS and that $S_w = 1 - S_g - S_o$, the derivatives of $k_{ro}$ are calculated as follows:

$$\frac{\partial k_{ro}}{\partial S_g} = \frac{\overline{k_{rog}} + S_g \dfrac{\partial \overline{k_{rog}}}{\partial S_g} - \overline{k_{row}} + (S_w - S_{wc}) \dfrac{\partial \overline{k_{row}}}{\partial S_g}}{1 - S_o - S_{wc}}$$

$$\frac{\partial \overline{k_{rog}}}{\partial S_g} = \frac{\partial k_{rog}(1 - S_o - S_{wc})}{\partial S_g} = -\frac{\partial k_{rog}}{\partial S_o}\frac{\partial S_o}{\partial S_g} = 0$$

$$\frac{\partial \overline{k_{row}}}{\partial S_g} = \frac{\partial \overline{k_{row}}}{\partial S_w}\frac{\partial S_g}{\partial S_w} = -\frac{\partial \overline{k_{row}}}{\partial S_w} = -\frac{\partial k_{row}}{\partial S_w}$$

$$\frac{\partial k_{ro}}{\partial S_g} = \frac{k_{rog} - k_{row} - (S_w - S_{wc})\dfrac{\partial k_{row}}{\partial S_w}}{1 - S_o - S_{wc}}$$

$$\frac{\partial k_{ro}}{\partial S_o} = \frac{(S_g \dfrac{\partial \overline{k_{rog}}}{\partial S_o} - \overline{k_{row}} + (S_w - S_{wc})\dfrac{\partial \overline{k_{row}}}{\partial S_o})(1 - S_o - S_{wc}) + (S_g \overline{k_{rog}} + (S_w - S_{wc})\overline{k_{row}})}{(1 - S_o - S_{wc})^2}$$

$$= \frac{k_{ro} + S_g \dfrac{\partial \overline{k_{rog}}}{\partial S_o} - \overline{k_{row}} + (S_w - S_{wc})\dfrac{\partial \overline{k_{row}}}{\partial S_o}}{1 - S_o - S_{wc}}$$

$$\frac{\partial \overline{k_{rog}}}{\partial S_o} = \frac{\partial k_{rog}(1 - S_o - S_{wc})}{\partial S_o} = -\frac{\partial k_{rog}}{\partial S_g}$$

$$\frac{\partial \overline{k_{row}}}{\partial S_o} = \frac{\partial \overline{k_{row}}}{\partial S_w}\frac{\partial S_w}{\partial S_o} = -\frac{\partial k_{row}}{\partial S_w}$$

$$\frac{\partial k_{ro}}{\partial S_o} = \frac{k_{ro} - S_g \dfrac{\partial k_{rog}}{\partial S_g} - k_{row} - (S_w - S_{wc})\dfrac{\partial k_{row}}{\partial S_w}}{1 - S_o - S_{wc}}$$

### 6.2.3   Normalized Baker model

In order to simulate thermal processes, Baker model was modified by using normalized saturations and relative permeabilities. We define normalized saturations and relative permeabilities as follows:

- Oil-Water system:

$$S_w^* = \frac{S_w - S_{wc}}{1 - S_{orw} - S_{wc}},$$

$$k_{rw}^*(S_w^*) = \frac{k_{rw}(S_w)}{k_{rwc}},$$

$$k_{row}^*(S_w^*) = \frac{k_{row}(S_w)}{k_{rowc}}.$$

- Gas-Oil system:

$$S_g^* = \frac{S_g - S_{gc}}{1 - S_{org} - S_{gc} - S_{wc}},$$

$$k_{rg}^*(S_g^*) = \frac{k_{rg}(S_g)}{k_{rgc}},$$

$$k_{rog}^*(S_g^*) = \frac{k_{rog}(S_g)}{k_{rogc}}.$$

N.B: For Baker interpolation to work, the two curves OW and GO on the saturation triangle must meet $=> S_{gc} = 0$ .

To be consistent with the previous Baker formulation, the normalized oil relative permeability is written as follows:

$$k_{ro}^*(S_w^*, S_g^*) = \frac{S_g^* \overline{k_{rog}^*} + S_w^* \overline{k_{row}^*}}{S_g^* + S_w^*},$$

$$k_{ro}^*(S_w^*, S_g^*) = \frac{S_g^{*,2P} \overline{k_{rog}^{*,3P}} + S_w^{*,2P} \overline{k_{row}^{*,3P}}}{S_g^{*,2P} + S_w^{*,2P}},$$

where the two-phase relative permeabilities are evaluated at the same normalized oil saturation:

$$\overline{k_{row}^{*,3P}} = k_{row}\left(\frac{(1 - S_o) - S_{wc}}{1 - S_{orw} - S_{wc}}\right),$$

$$\overline{k_{rog}^{*,3P}} = k_{rog}\left(\frac{(1 - S_o - S_{wc}) - S_{gc}}{1 - S_{org} - S_{gc} - S_{wc}}\right),$$

The upper-scripts $2P$ and $3P$ indicate how the different quantities are evaluated.

To be consistent with the definition of $k_{rw}^*$ and $k_{rg}^*$, we assume that $k_{ro}^* = \frac{k_{ro}(S_w, S_g)}{k_{roc}}$, where $k_{roc}$ will be defined later. Moreover for the rescaling to work, we have to assume that $k_{row}(S_w = S_{wc}) = k_{rog}(S_g = S_{gc})$ (see Stone's Three-Phase Model I).
Finally, we get $k_{roc} = k_{row}(S_w = S_{wc}) = k_{rog}(S_g = S_{gc}) = k_{ro\alpha c}$, $\alpha = w, g$ .

We can then rescale $k_{ro}^*(S_w^*, S_g^*)$ to get $k_{ro}(S_w, S_g)$ and get its derivatives:

$k_{ro}(S_w, S_g) = k_{ro\alpha c} k_{ro}^*(S_w^*, S_g^*)$

$\dfrac{\partial k_{ro}}{\partial S_g} = k_{ro\alpha c} \dfrac{\partial k_{ro}^*}{\partial S_g}$

$\dfrac{\partial k_{ro}}{\partial S_o} = k_{ro\alpha c} \dfrac{\partial k_{ro}^*}{\partial S_o}$

### 6.2.4 Derivatives of $k_{ro}$ with respect to saturation

To make it more readable, we removed the $\bar{\phantom{x}}$ and the $^*$ from the different quantities.

$$\frac{\partial k_{ro}^*}{\partial S_g} = \frac{(\frac{\partial S_g^{2P}}{\partial S_g}k_{rog}^{3P} + S_g^{2P}\frac{\partial k_{rog}^{3P}}{\partial S_g} + \frac{\partial S_w^{2P}}{\partial S_g}k_{row}^{3P} + S_w^{2P}\frac{\partial k_{row}^{3P}}{\partial S_g})(S_g^{2P} + S_w^{2P}) - (S_g^{2P}k_{rog}^{3P} + S_w^{2P}k_{row}^{3P})\frac{\partial(S_g^{2P} + S_w^{2P})}{\partial S_g}}{(S_g^{2P} + S_w^{2P})^2}$$

$$\frac{\partial k_{ro}^*}{\partial S_g} = \frac{(\frac{\partial S_g^{2P}}{\partial S_g}k_{rog}^{3P} + S_g^{2P}\frac{\partial k_{rog}^{3P}}{\partial S_g} + \frac{\partial S_w^{2P}}{\partial S_g}k_{row}^{3P} + S_w^{2P}\frac{\partial k_{row}^{3P}}{\partial S_g}) - k_{ro}^*\frac{\partial(S_g^{2P} + S_w^{2P})}{\partial S_g}}{S_g^{2P} + S_w^{2P}}$$

Intermediate calculations:

$$\frac{\partial k_{rog}^{3P}}{\partial S_g} = 0, \text{see definition of } k_{rog}^{3P}$$

$$\frac{\partial k_{row}^{3P}}{\partial S_g} = \frac{\partial k_{row}^{3P}}{\partial S_w^{2P}}\frac{\partial Sw^{2P}}{\partial S_w}\frac{\partial S_w}{\partial S_g}$$

$$\frac{\partial Sw^{2P}}{\partial S_w} = \frac{1}{1 - S_{orw} - S_{wc}} = \frac{1}{\alpha_1}$$

$$\frac{\partial Sg^{2P}}{\partial S_g} = \frac{1}{1 - S_{org} - S_{gc} - S_{wc}} = \frac{1}{\alpha_2}$$

Result:

$$\frac{\partial k_{ro}^*}{\partial S_g} = \frac{\frac{1}{\alpha_1}(k_{rog}^{3P} - k_{ro}^*) - \frac{1}{\alpha_2}(k_{row}^{3P} + S_w^{2P}\frac{\partial k_{row}^{3P}}{\partial S_w^{2P}} - k_{ro}^*)}{S_g^{2P} + S_w^{2P}}$$

$$\frac{\partial k_{ro}}{\partial S_g} = k_{ro\alpha c}\frac{\partial k_{ro}^*}{\partial S_g}$$

$$\frac{\partial k_{ro}^*}{\partial S_o} = \frac{(\frac{\partial S_g^{2P}}{\partial S_o}k_{rog}^{3P} + S_g^{2P}\frac{\partial k_{rog}^{3P}}{\partial S_o} + \frac{\partial S_w^{2P}}{\partial S_o}k_{row}^{3P} + S_w^{2P}\frac{\partial k_{row}^{3P}}{\partial S_o}) - k_{ro}^*\frac{\partial(S_g^{2P} + S_w^{2P})}{\partial S_o}}{S_g^{2P} + S_w^{2P}}$$

$$\frac{\partial k_{ro}^*}{\partial S_o} = \frac{-\frac{1}{\alpha_1}S_g^{2P}\frac{\partial k_{rog}^{3P}}{\partial S_g^{2P}} - \frac{1}{\alpha_2}(k_{row}^{3P} + S_w^{2P}\frac{\partial k_{row}^{3P}}{\partial S_w^{2P}} - k_{ro}^*)}{S_g^{2P} + S_w^{2P}}$$

$$\frac{\partial k_{ro}}{\partial S_o} = k_{ro\alpha c}\frac{\partial k_{ro}^*}{\partial S_o}$$

### 6.2.5 Validation of the model with $S_{orw} = S_{org} = S_\alpha$

NB: $k^*_{row}(f^*) = \dfrac{k_{row}(f)}{k_{ro\alpha c}}$.

$$\overline{k_{row}} = k_{row}(1 - S_o),$$
$$= k^*_{row}((1 - S_o)^*)k_{ro\alpha c},$$
$$= k_{row}\left(\frac{(1 - S_o) - S_{wc}}{1 - S_\alpha - S_{wc}}\right)k_{ro\alpha c},$$
$$= \overline{k^*_{row}}k_{ro\alpha c}.$$

$$k_{ro}(S_w, S_g) = \frac{S_g\overline{k_{rog}} + (S_w - S_{wc})\overline{k_{row}}}{S_g + (S_w - S_{wc})} \iff k_{ro}(S_w, S_g) = \frac{(1 - S_\alpha - S_{wc})S^*_g\overline{k_{rog}} + (1 - S_\alpha - S_{wc})S^*_w\overline{k_{row}}}{(1 - S_\alpha - S_{wc})(S^*_g + S^*_w)}$$

$$\iff k_{ro}(S_w, S_g) = \frac{S^*_g\overline{k^*_{rog}}k_{ro\alpha c} + S^*_w\overline{k^*_{row}}k_{ro\alpha c}}{S^*_g + S^*_w}$$

$$\iff \frac{k_{ro}(S_w, S_g)}{k_{ro\alpha c}} = k^*_{ro}.$$

### 6.2.6 Steps of the implementation for the normalized Baker model

- get saturation and relative permeability endpoints respecting the requirements of the method: $S_{gc} = 0$, $k_{ro\alpha c} = k_{row}(S_w = S_{wc}) = k_{rog}(S_g = S_{gc})$ (enter input data accordingly),

- calculate normalized saturations and two-phase relative permeabilities,

- calculate normalized oil relative permeability,

- rescale oil relative permeability.

### 6.2.7 Example of input data

Input data are entered such that:
- for an oil-water system:

- $S_w \in [S_{wc}; 1 - S_{orw}]$,

- $k_{rw} \in [0; k_{rwc}]$,

- $k_{row} \in [0; k_{rocw}]$.

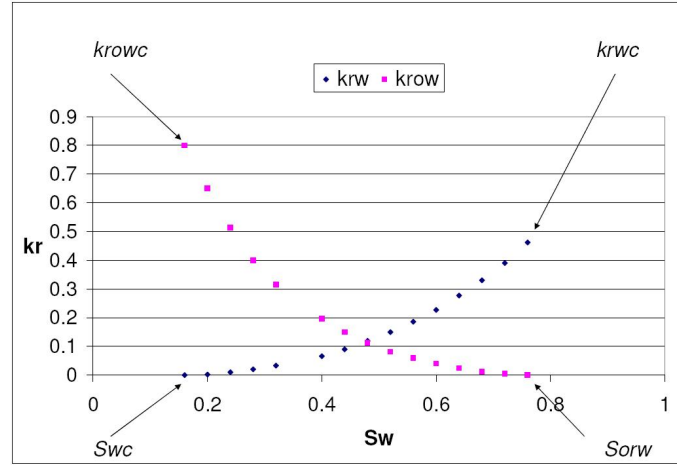Figure 3: Two-phase input data: oil-water system

- for a gas-oil system:

- $S_g \in [0; 1 - S_{org} - S_{wc}]$,

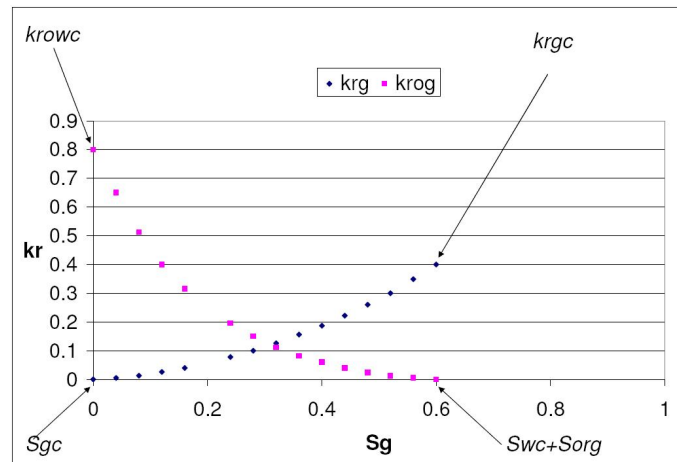- $k_{rg} \in [0; k_{rgc}]$,

- $k_{rog} \in [0; k_{rocw}]$.



Figure 4: Two-phase input data: gas-oil system

We define the three-phase equilibrium to set initial saturations, as follows:
- in the water zone:

- $S_g = 0$,

- $S_o = 0$,

- $S_w = 1$.

- in the oil zone:

- $S_g = 0$,

- $S_o = 1 - S_{wc}$,

- $S_w = S_{wc}$.

- in the gas zone:

- $S_g = 1 - S_{org} - S_{wc}$,

- $S_o = S_{org}$,

- $S_w = S_{wc}$.

### 6.2.8 Different test cases

We ran the following test cases in order to validate the normalized model:

- $S_{wc} = S_{orw} = S_{org} = 0$ and all values normalized (so that both codes calculate the same thing). In that case, we must enter a minimal value for $S_{wc}$ (=1E-5) to set the three-phase equilibrium.

- $S_{orw} = S_{org}$. Again both codes calculate the same oil relative permeability (see proof above).

We then tried different sets of saturations (verifying the following constraint: $S_w + S_g + S_o = 1$) and found logical values of the three-phase relative permeability. See also (see Figure **??**) for testing on derivatives.

## 6.3 Temperature dependent endpoints

Although neglected in first approximation, it is important to consider that saturation and relative permeabilities endpoints depend on temperature when it comes to run thermal simulations.

### 6.3.1 Water saturation endpoints

In this paragraph, we only study the influence of temperature on the critical water saturation. We assume a linear dependency between $S_{wc}$ and $T$:

$S_{wc}(T) = S_{wc}^0 + \alpha \Delta T$
or
$S_{wc}(T) = S_{wc}^0 + S_{wcT}$

$S_{wc}^0$ is the initial water saturation,
$\alpha$ is a coefficient, positive, negative or equal to zero,
$\Delta T = T - T^0$.

Depending on the sign of $S_{wcT}$, we have to consider 3 different cases:

- $S_{wcT} < 0$, then $S_{wc}(T)$ decreases and the water flows more easily,

- $S_{wcT}$, then it comes to study the isothermal case,

- $S_{wcT} > 0$, then $S_{wc}(T)$ increases and the water flows less easily.

We will illustrate these three cases in the following testings.

### 6.3.2 Derivatives of $k_{ro}$ with respect to temperature

We can then calculate:

$$\frac{\partial k_{rw}}{\partial T} = \frac{\partial k_{rw}}{\partial S_{wc}}\frac{\partial S_{wc}}{\partial T}$$

$$\frac{\partial k_{rw}}{\partial T} = \alpha\frac{\partial k_{rw}}{\partial S_{wc}}$$

Intermediate calculations:

$$\frac{\partial k_{rw}}{\partial S_{wc}} = k_{rwc}\frac{\partial k_{rw}^*}{\partial S_w^{2P}}\frac{\partial Sw^*}{\partial S_{wc}}$$

$$Sw^* = Sw^{2P}$$

$$\frac{\partial Sw^*}{\partial S_{wc}} = \frac{S_w + S_{orw} - 1}{(1 - S_{orw} - S_{wc})^2} = \alpha_4$$

Result:

$$\frac{\partial k_{rw}}{\partial T} = \alpha\alpha_4 k_{rwc}\frac{\partial k_{rw}^*}{\partial S_w^{2P}}$$

$$\frac{\partial k_{rg}}{\partial T} = \frac{\partial k_{rg}}{\partial S_{wc}}\frac{\partial S_{wc}}{\partial T}$$

$$\frac{\partial k_{rg}}{\partial T} = \alpha\frac{\partial k_{rg}}{\partial S_{wc}}$$

Intermediate calculations:

$$\frac{\partial k_{rg}}{\partial S_{wc}} = k_{rgc}\frac{\partial k_{rg}^*}{\partial S_g^{2P}}\frac{\partial Swg^*}{\partial S_{wc}}$$

$$Sg^* = Sg^{2P}$$

$$\frac{\partial Sg^*}{\partial S_{wc}} = \frac{S_g + S_{gc}}{(1 - S_{org} - S_{gc} - S_{wc})^2} = \alpha_3$$

Result:

$$\frac{\partial k_{rg}}{\partial T} = \alpha\alpha_3 k_{rgc}\frac{\partial k_{rg}^*}{\partial S_g^{2P}}$$

$$\frac{\partial k_{ro}}{\partial T} = \frac{\partial k_{ro}}{\partial S_{wc}}\frac{\partial S_{wc}}{\partial T}$$

$$\frac{\partial k_{ro}}{\partial T} = \alpha\frac{\partial k_{ro}}{\partial S_{wc}}$$

Intermediate calculations:

$$\frac{\partial k_{ro}}{\partial S_{wc}} = \frac{\left(\dfrac{\partial S_g^{2P}}{\partial S_{wc}}k_{rog}^{3P} + S_g^{2P}\dfrac{\partial k_{rog}^{3P}}{\partial S_{wc}} + \dfrac{\partial S_w^{2P}}{\partial S_{wc}}k_{row}^{3P} + S_w^{2P}\dfrac{\partial k_{row}^{3P}}{\partial S_{wc}}\right) - k_{ro}^*\dfrac{\partial (S_g^{2P} + S_w^{2P})}{\partial S_{wc}}}{S_g^{2P} + S_w^{2P}}$$

$$\frac{\partial k_{ro}}{\partial S_{wc}} = \frac{\alpha_3\left(k_{rog}^{3P} + S_g^{2P}\dfrac{\partial k_{rog}^{3P}}{\partial S_g^{2P}} - k_{ro}^*\right) + \alpha_4\left(k_{row}^{3P} + S_w^{2P}\dfrac{\partial k_{row}^{3P}}{\partial S_w^{2P}} - k_{ro}^*\right)}{S_g^{2P} + S_w^{2P}}$$

# 7   Appendix A: thermal I/O in GPRS

In this section we present the way to provide thermal information for GPRS.

## 7.1   FLUID_TYPE

For fluid type we introduce new postfix for type of the model. User can specified postfix _THERMAL for both fluid type model BLACK_OIL or COMPOSITIONAL. This postfix show that simulator have to switch into thermal regime and thermal keywords expected.

---
**Example**
`BLACK_OIL_THERMAL`

---

---
**Example**
`COMPOSITIONAL_THERMAL`

---

## 7.2   PVTT

If FLUID_TYPE keyword specified thermal postfix for black-oil type of model (BLACK_OIL_THERMAL), GPRS expect thermal PVT table to be presented right after standard isothermal PVT table for each of phase. First two fields for this keyword are reference pressure PREF and reference temperature TREF for both tables (see section 2.3). Here $T_{ref}$ is also used as default temperature for introduced isothermal PVT table.

Next needs to be specified number of rows in table NUM_OF_TABLE_ENTRIES and table itself.

The first column in table is values of temperature, the second column - formation volume factor values, the third - values of viscosity and the last forth - specific heat values. All formulae for calculation of black-oil properties as function of introduced parameters presented in section 2.3.

---
**Example**
```
BLACK_OIL_THERMAL
...
PREF 3014.7
TREF 600
NUM_OF_TABLE_ENTRIES 6
 # T(R)   Bo(RB/STB)  VISC(cP)   SPECH(SCF/STB)
 500      0.970006    23.0       0.5
 600      0.970006    18.0       0.5
 700      0.970006    7.0        0.5
 800      0.970006    3.0        0.5
 900      0.970006    2.0        0.5
 1000     0.970006    1.0        0.5
```

---

## 7.3   ENTHALPY

In case FLUID_TYPE keyword specified thermal compositional model (COMPOSITIONAL_THERMAL) GPRS expect polynomial coefficients to be presented right between binary interaction coefficients and PVT table for water (PVTW). So far we use linear approximation for enthalpy as function of temperature (see 3.2.2). Two rows contained enthalpy coefficients for each component need to be presented.

**Example**
```
COMPOSITIONAL_THERMAL
NPHASES 2
NCOMPONENTS 4
...
 # A coef  (free)
 -35.1094  -28.0629  -28.1694  -28.1694
 # B coef  (linear)
 0.2704    0.2384    0.2416    0.2416
```

## 7.4  ROCK_DATA

For thermal black-oil model we also need to specify rock specific heat capacity and reference temperature in order to calculate internal energy for rock (see 2.3). We add these parameters to word ROCK_DATA. Instead of two parameters this keyword introduce four parameters for thermal model - compressibility $c_R$, reference pressure $p_{ref}$, specific heat capacity $C_R$ and reference temperature $T_{ref}$.

**Example**
```
ROCK_DATA
 # COMP.  P.REF  SPECR  T.REF
  3.E-6   14.7    10     500
```

## 7.5  WCONINJE

For well control several temperature based controls for injection well were added. So far only two types of thermal controls added. It is BHPT for bottom hole pressure control thermal injection and WRATET for water rate control thermal injection.

The only difference from isothermal controls is the last field for temperature specification. Below you can find examples of using these keywords.

**Example**
```
#COMPDAT
number_of_connections 1
 # LOC(ijk)  WI
 24          966.302
END
#WCONINJE
 # CTRL  BHP  NC  z1    z2    z3    z4    T
 BHPT    600  4   1.0   0.0   0.0   0.0  600
END
```

**Example**
```
#COMPDAT
number_of_connections 1
 # LOC(ijk)  WI
 9           9130
END
#WCONINJE
 # CTRL  BHP    RATE     dens   NC  z1  z2  z3  T
 WRATET  2000  1000.0   64.79   3   0   0   1   540
END
```

# 8 Appendix B: several correlations

In this chapter, we gathered some information about water, steam and hydrocarbon properties in compositional, validation tests on oil and water properties in black-oil and testing on relative permeability derivatives.

## 8.1 Water phase properties in compositional

We take the description given by [17] pp.861-863.

### 8.1.1 Water density

The water density (in lbm/cuft) is given with $T$ in R and $P$ in psi by

$$\rho_w = \frac{\rho_{\text{ref},w}}{[1 - c_{Pw}(P - P_{\text{ref}})][1 + c_{T1}(T - T_{\text{ref}}) + c_{T2}(T - T_{\text{ref}})^2]}$$

where the reference density is given by

$$\rho_{\text{ref},w} = \frac{\rho_{s,w}}{B_w(P_{\text{ref}})}$$

and

| | |
|---|---|
| $\rho_{s,w}$ | is the water density at surface conditions |
| $P_{\text{ref}}$ | is the reference pressure given by the standard conditions |
| $B_w(P_{\text{ref}})$ | is the formation volume factor at the reference pressure ($= 1$) |
| $c_{Pw}$ | is the water compressibility ($= 3 \times 10^{-6}(1/\text{psi})$) |
| $T_{\text{ref}}$ | is the reference temperature given by the standard conditions |
| $c_{T1}$ | is the first coefficient of thermal expansion ($= 1.67 \times 10^{-4}\text{R}^{-1}$) |
| $c_{T2}$ | is the second coefficient of thermal expansion ($= 9.26 \times 10^{-7}\text{R}^{-2}$). |

All the values given are the default values taken from [17].

The water density is clearly a function of $P$ and $T$; we can then calculate the derivatives with respect to $P$ and $T$:

$$\frac{\partial \rho_w}{\partial P} = \rho_w \frac{c_{Pw}}{[1 - c_{Pw}(P - P_{\text{ref}})]}$$

and

$$\frac{\partial \rho_w}{\partial T} = -\rho_w \frac{c_{T1} + 2(T - T_{\text{ref}})c_{T2}}{[1 + c_{T1}(T - T_{\text{ref}}) + c_{T2}(T - T_{\text{ref}})^2]}.$$

### 8.1.2 Water viscosity

The water viscosity (in cP) is given by the following correlation:

$$\mu_w = \frac{1}{A_w + B_w T_c + C_w T_c^2}$$

where

| | |
|---|---|
| $T_c$ | is the temperature in C |
| $A_w, B_w, C_w$ | are derived coefficients |
| $A_w$ | $= 0.1323$ |
| $B_w$ | $= 0.03333$ |
| $C_w$ | $= 7.643 \times 10^{-6}$. |

The water viscosity is a temperature dependent function; we get:

$$\frac{\partial \mu_w}{\partial P} = 0$$

and

$$\frac{\partial \mu_w}{\partial T} = -\mu_w^2 (B_w - 2C_w T_c).$$

### 8.1.3  Enthalpy and internal energy

We take the description given by [11] pp.278-282. We define three quantities as a function of temperature:

- heat capacity in a liquid phase $C_{pl}(T)$ in Btu/lbmol-R (cal/gmol-K),

- heat capacity in the gas phase $C_{pg}(T)$ in Btu/lbmol-R (cal/gmol-K), and

- enthalpy of vapourization $H_{vap}(T)$ in Btu/lbmol.

$T$ unit is R.
These three quantities are related by the following definition:

$$H_{vap}(T) = H_g(T) - H_l(T),$$

where

- $H_l(T)$ is the component enthalpy in a liquid phase defined by $C_{pl}(T) = \dfrac{dH_l(T)}{dT}$,

- $H_g(T)$ is the component enthalpy in the gas phase defined by $C_{pg}(T) = \dfrac{dH_g(T)}{dT}$.

Condensable components :

$$C_{pg}(T) = C_{pg1} + C_{pg2}T + C_{pg3}T^2 + C_{pg4}T^3$$
$$H_{vap}(T) = H_{vr}(T_{crit} - T)^{ev}.$$

The component vapour enthalpy $H_g(T)$ is the integral of $C_{pg}(T)$ from $T_{ref}$ to $T$.
Enthalpy datum is gas phase at $T = T_{ref}$
The component liquid enthalpy is $H_l(T) = H_g(T) - H_{vap}(T)$.

Non-condensable components ($T > T_{crit}$):

$$C_{pg}(T) = C_{pg1} + C_{pg2}T + C_{pg3}T^2 + C_{pg4}T^3$$

The component vapour enthalpy $H_g(T)$ is the integral of $C_{pg}(T)$ from $T_{ref}$ to $T$.

Two correlations are available to evaluate $C_{pg}$:

- the four-coefficient correlation uses:
  $C_{pg1} = 7.701$, $C_{pg2} = 2.553 \times 10^{-4}$, $C_{pg3} = 7.781 \times 10^{-7}$, $C_{pg4} = -1.473 \times 10^{-10}$

- the two-coefficient correlation uses:
  $C_{pg1} = 7.613$, $C_{pg2} = 8.616 \times 10^{-4}$.

The four-coefficient correlation is the most accurate.

The enthalpy and the internal energy in the water phase are defined by

$$H_w(T) = \sum_{i=1}^{n_c} w_i \times H_{l,i}(T)$$

$$U_w(T) = H_w(T) - \frac{P_w}{\rho_w}$$

where

$w_i$    is the mol fraction of component $i$ in the water phase
$P_w$    is the water phase pressure defined by
     $P_w = P_g - P_{cgo}(S_g) - P_{cwo}(S_w)$, if we take the capillary pressure effect into account,
     $P_w = P_g = P$, if not.
$\rho_w$    is the water phase mole density.

We consider that the water component is the only component present in the water phase; we end up with:

$$H_w(T) = H_l(T)$$

$$U_w(T) = H_w(T) - \frac{P_w}{\rho_w}.$$

Their derivatives are defined by:

$$\frac{dH_w(T)}{dT} = \frac{dH_l(T)}{dT}$$

and

$$\frac{dU_w(T)}{dT} = \frac{dH_w(T)}{dT} + \frac{\partial \rho_w}{\partial T} \frac{P_w}{\rho_w^2}$$

with

$$\frac{dH_l(T)}{dT} = \frac{dH_g(T)}{dT} - \frac{dH_{vap}(T)}{dT}$$

$$\frac{dH_g(T)}{dT} = C_{pg}(T)$$

$$\frac{dH_{vap}(T)}{dT} = -ev \times H_{vr}(T_{crit} - T)^{ev-1} \text{ if } T > T_{crit},$$

$$\frac{dH_{vap}(T)}{dT} = 0 \text{ if } T < T_{crit}.$$

## 8.2   Steam properties in compositional

### 8.2.1   Steam density

The steam density is calculated from the real gas law:

$$\rho_{\text{steam}} = \rho_{\text{steam},b}\frac{T_b}{T}$$

where $T_b$ is the boiling point temperature and $\rho_{\text{steam},b}$ is the density at the boiling point. The saturated water vapor density is given by

$$\rho_{\text{steam},b} = \exp[C_0 + C_1 T_b + C_2 T_b^2 + C_3 T_b^3 + C_4 T_b^4 + C_5 T_b^5]$$

where, $\rho_{\text{steam},b}$ is in lbmol/cuft, $T_b$ is the boiling point temperature in K and

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $C_0$ | = | -93.7072 | $C_1$ | = | 0.833941 | $C_2$ | = | -0.003208 |
| $C_3$ | = | $6.57652 \times 10^{-6}$ | $C_4$ | = | $-6.93747 \times 10^{-9}$ | $C_5$ | = | $2.97203 \times 10^{-12}$. |

The derivatives are given by:

$$\frac{\partial \rho_{\text{steam}}}{\partial P} = 0$$

and

$$\frac{\partial \rho_{\text{steam}}}{\partial T} = -\frac{\rho_{\text{steam}}}{T}.$$

### 8.2.2   Steam viscosity

The steam viscosity is given by:

$$\mu_{\text{steam}} = A_g + B_g T_c + C_g P_p^{D_g}$$

where the temperature $T_c$ is in °C, the pressure $P_p$ is in MPa
and $A_g = 4.9402 \times 10^{-3}$, $B_g = 5.0956 \times 10^{-5}$, $C_g = 2.9223 \times 10^{-6}$, $D_g = 2.5077$.

The derivatives are:

$$\frac{\partial \mu_{\text{steam}}}{\partial P} = C_g D_g P_p^{D_g - 1}$$

and

$$\frac{\partial \mu_{\text{steam}}}{\partial T} = B_g.$$

## 8.3 Hydrocarbon properties in compositional

In this paragraph, we present the derivatives of viscosity.

$$\frac{\partial \mu^*}{\partial x_i} = (\mu_i^* - \mu) \frac{\sqrt{M_i}}{\sum\limits_{i=1}^{n_c} (x_i \sqrt{M_i})}$$

$$\frac{\partial \mu^*}{\partial T} = \frac{\sum\limits_{j=1}^{n_c} (x_j \frac{\partial \mu_j^*}{\partial T} \sqrt{M_j})}{\sum\limits_{j=1}^{n_c} (x_j \sqrt{M_j})}$$

with

$$\frac{\partial \mu_j^*}{\partial T} = 0.94 \frac{\mu_j^*}{T}, (T_{rj} < 1.5),$$

$$\frac{\partial \mu_j^*}{\partial T} = 4.58 \frac{5}{8} \mu_j^* \frac{1}{T_{cj}(4.58 T_{rj} - 1.67)}, (T_{rj} > 1.5),$$

$$\frac{\partial \mu}{\partial x_i} = \frac{\partial \mu^*}{\partial x_i} + \frac{4}{\zeta} \left( \rho V_{ci} + \frac{1}{\rho_c} \frac{\partial \rho}{\partial x_i} \right) (A + B\rho_r + C\rho_r^2 - D\rho_r^3 + E\rho_r^4)^3 (B + 2C\rho_r - 3D\rho_r^2 + 4E\rho_r^3)$$

$$- \frac{1}{\zeta} \left( (A + B\rho_r + C\rho_r^2 - D\rho_r^3 + E\rho_r^4)^4 - 1 \times 10^{-4} \right) \left( \frac{1}{6} \frac{T_{ci}}{\sum\limits_{j=1}^{n_c}(x_j T_{cj})} - \frac{1}{2} \frac{M_i}{\sum\limits_{j=1}^{n_c}(x_j M_j)} - \frac{2}{3} \frac{P_{ci}}{\sum\limits_{j=1}^{n_c}(x_j P_{cj})} \right)$$

$$\frac{\partial \mu}{\partial P} = \frac{4}{\zeta \rho_c} (A + B\rho_r + C\rho_r^2 - D\rho_r^3 + E\rho_r^4)^3 (B + 2C\rho_r - 3D\rho_r^2 + 4E\rho_r^3) \frac{\partial \rho}{\partial P}$$

$$\frac{\partial \mu}{\partial T} = \frac{\partial \mu^*}{\partial T} + \frac{4}{\zeta \rho_c} (A + B\rho_r + C\rho_r^2 - D\rho_r^3 + E\rho_r^4)^3 (B + 2C\rho_r - 3D\rho_r^2 + 4E\rho_r^3) \frac{\partial \rho}{\partial T}.$$

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