International Research Training Group nupus

Phase transitions as non-linear complementarity problems

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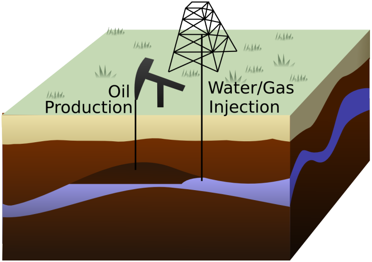
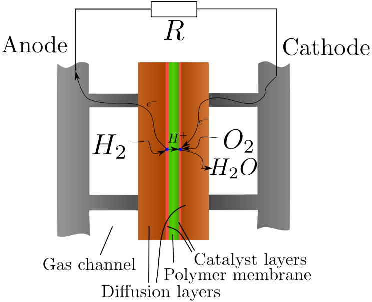
Motivation





- Miscible multi-phase fluid systems have many significant applications
- Difficulties of numerical simulations for those thermodynamic systems are much larger than if assuming immiscibility
- One reason for these difficulties are phase transitions, i.e., the appearance or disappearance of a fluid
- A sound approach is desirable

Overview

1. Flash Calculations

2. Flow Models

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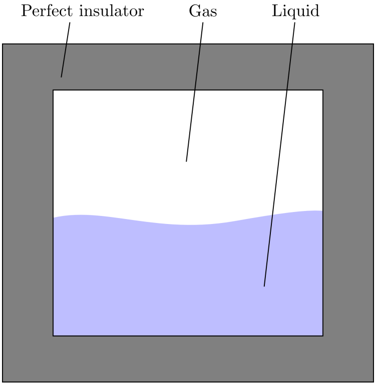
Flash Calculations



Given Quantities:

- Temperature T
- Total concentration of every component $c_{tot}^{\kappa} := \sum_{\alpha} c_{\alpha}^{\kappa} S_{\alpha}$

Desired Quantities:

- Pressures p_{α}
- Phase Compositions $\{x_{\alpha}^{\kappa}\}$
- Phase Saturations S_{α}

Overall:

- $M \cdot N + 2 \cdot M$ unknowns for M phases, N components
- We need the same number of equartions

Equations

Assume thermodynamic equilibrium:

- Thermal Equilibrium: All phase temperatures are equal, i.e., $T_\alpha = T_\beta = T$ (Does not count: We implicitly assumed that there is only one temperature)
- Mechanical Equilibrium: All phase pressures are equal, i.e., $p_\alpha = p_\beta$ (In porous media: Difference between phase pressures is capillary pressure, i.e., $p_\alpha - p_\beta = p_{\mathrm{c},\alpha\beta}$)
- Chemical Equilibrium: All component fugacities are the same in all phases, i.e., $f_\alpha^\kappa = f_\beta^\kappa = f^\kappa$, where

$$f_\alpha^\kappa =: \phi_\alpha^\kappa x_\alpha^\kappa p_\alpha$$

- Overall: $(N + 1) \cdot (M - 1)$ independent relations
- $N + M + 1$ further equations necessary

Equations [cont]

- Closure condition for saturations: $\sum_\alpha S_\alpha = 1$
- Definition of total component concentration: $c^\kappa_{tot} := \sum_\alpha c^\kappa_\alpha S_\alpha$; with $c^\kappa_\alpha := \rho_{\mathrm{mol},\alpha} x^\kappa_\alpha$ and with $\rho_{\mathrm{mol},\alpha}$ defined by the equation of state of phase α
- M equations still missing $\Longrightarrow$ Model assumptions

Model assumptions

We use NCP functions to specify the model assumptions:

- Phase α can only be present if its “mole fractions” x_α^κ sum up to one:

$$\sum_\kappa x_\alpha^\kappa = 1 \implies S_\alpha \geq 0$$

- If the sum of the “mole fractions” x_α^κ is smaller than 1, the phase cannot be present:

$$S_\alpha = 0 \implies \sum_\kappa x_\alpha^\kappa \leq 1$$

- A fluid phase is always either present or not, i.e., one of the above two equalities is true.
- Leads to the non-linear complementarity problem (NCP):

$$S_\alpha \left(1 - \sum_\kappa x_\alpha^\kappa \right) = 0 \wedge S_\alpha \geq 0 \wedge 1 - \sum_\kappa x_\alpha^\kappa \geq 0$$

Model assumptions [cont]

- Can be directly embedded in the system of equations using a non-linear complementarity function $\Phi_\alpha : \mathbf{R}^2 \rightarrow \mathbf{R}$.
- All Φ exhibit the property

$$\Phi_\alpha(a, b) = 0 \iff a \cdot b = 0 \wedge a \geq 0 \wedge b \geq 0$$

- In our case $a = S_\alpha$ and $b = 1 - \sum_\kappa x_\alpha^\kappa$
- Multiple choices for Φ_α are possible, the most simple is min.

Other Approaches

Other approaches have been proposed:

- Primary variable switching: exchange unphysical primary variables by ones which make sense physically (e.g. replace negative saturations by a fugacity)
- Negative saturations approach: Calculate the composition for all phases being potentially present, subtract the mass of “negative” saturations from the physically present phases
- Specialized models, e.g. the black-oil model

All these approaches have specific advantages and disadvantages.

Overview

1. Flash Calculations

2. Flow Models

Flash-Based Flow Models

- Use the component concentrations (mass per volume) as primary variables
- Calculate thermodynamic state using flash calculations
- Determine the residual and its JACOBIAN using the thermodynamic state

Disadvantage

- Flash solver needs to be very acurate to determine the residual's JACOBIAN if using finite differences
    - Implies high computational cost and leads to problems with IEEE 754 double precision floating point represenation
- Other approach should be used for implicit models

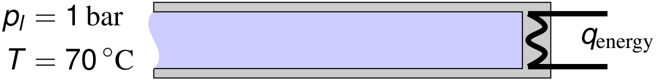
NCP Flow-Model

- Use fugacity f^κ of each component and saturation of each phase S_α as primary variables
- Calculate thermodynamic state from these
- Evaluate the balance and the NC-functions using the thermodynamic state

Benefits and Drawbacks

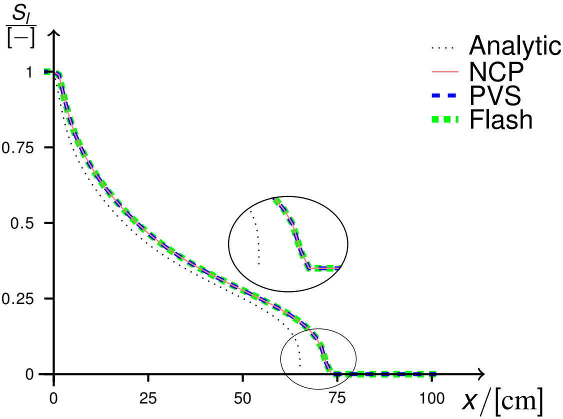
- Requires M additional primary variables/equations for the residual
    - Local assembly cost goes from $O((k \cdot N)^2)$ to $O((k \cdot (M + N))^2)$ (k is the number of degrees of freedom of an interaction entity)
- Empirically more stable than alternative approaches like primary variable switching
- Much easier to implement than primary variable switching
- Second item often offsets the first

Example: The Heat-Pipe Problem



- Quasi one-dimensional domain
- Domain closed to energy and mass everywhere except on the left
- Heated at constant rate at the right
- Leads to two-phase region in the middle
    - Counter-current mass flow
    - Evaporation and condensation
- Semi-analytical steady-state solution known

Heat-Pipe: Physical results



Liquid saturation using 100 line segments for spatial discretization

Heat-Pipe: Computational Performance

	NCP	PVS	Flash
Time steps	42	419	297
NEWTON iterations	210	4741	1645
CPU time $[\mathrm{s}]$	0.97	18.13	1924[1]

Effort for the numerical models to reach steady-state ($t = 10^9\ \mathrm{s}$)

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[1] Requires quadruple precision scalars

Implementation Complexity

	NCP	PVS	Flash
SLOC	551	720	621

Lines of code to implement the models in eWoms (excluding most of the boiler-plate code)

Conclusions

- NCP functions are empirically more stable than the primary variable switching approach
- Implementing a flash solver is not terribly hard when utilizing NCP functions
- Flash-based approaches can be used for implicit flow models, but are not very suited because of numerical precision issues and computational cost

Overview

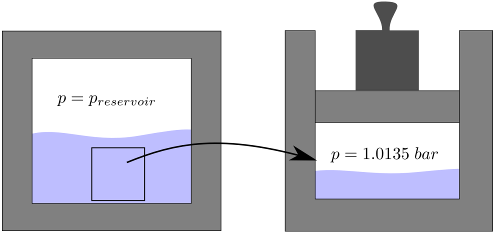
3 Black-Oil-Parameter Determination

The Black-Oil Model

Given a certain volume of oil at reservoir conditions, find

- Oil/gas density in the reservoir and at the surface
- Amount of gas per oil produced at the surface
- Oil composition in the reservoir

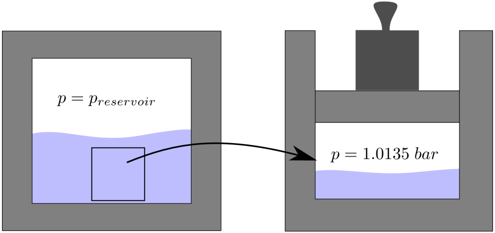
The Black-Oil Model



For this, the Black-Oil model uses the following parameters:

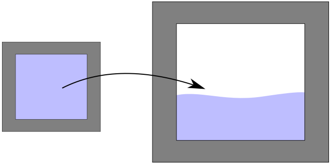
- Oil/Gas Formation Volume Factors (B_o, B_g): Ratio between density of oil/gas phase at reservoir pressure to density at surface condition
- Gas Formation Factor (R_s): Gas volume at surface that emerges from a given volume of oil at reservoir pressure

The Black-Oil Parameters



- The oil phase in the reservoir is a mixture two pseudo components, gas and oil
- The oil phase at the surface only consists of the oil component
- The reservoir is isothermal
- The composition of the two pseudo components is fixed for all pressures (i.e., their molar mass does not change)

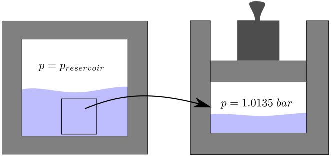
Volume Factors



Procedure to calculate the volume factors:

- Given: Initial oil composition, pressure, temperature, saturation
- Calculate the total component concentrations $c^{\kappa}_{tot} = \frac{m^{\kappa}_{tot}}{V}$
- Gradually increase the volume V of the vessel by dividing the total concentrations by a *reservoir relaxation factor* α_r
- For each value of the total concentration, execute a flash calculation and calculate the density of the gas and oil phases
    - Yields B_o and B_g dependant on pressure

Gas Formation Factor



Bring of the "relaxed" oil to the surface:

- Requires: Calculation of a *surface relaxation factor* α_s which is defined that by $p = 1.0135\,\mathrm{bar}$ when using α_s on the "relaxed oil" in the flash calculation
- Start with $\{c^{\kappa}_{tot} = x^{\kappa}_{r,o}\rho_{mol,o}\}$
- Use NEWTON-RAPHSON method to find α_s
  - Each NEWTON-RAPHSON step requires two flash calculations
- Gas formation factor is given by:

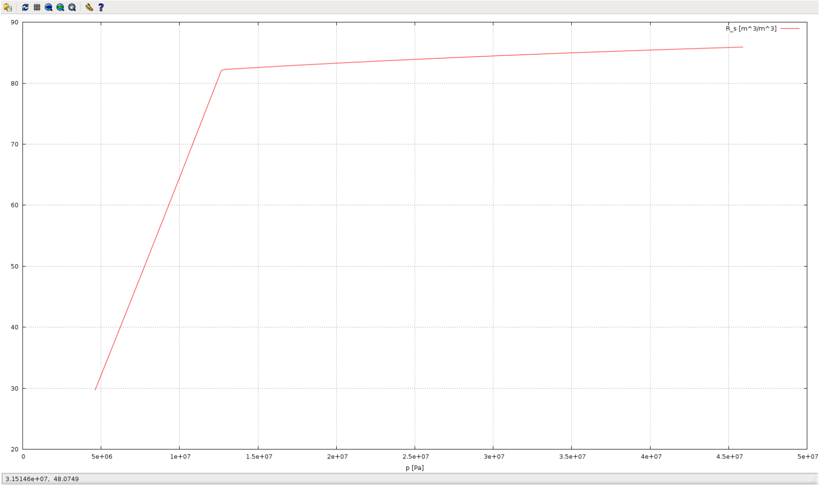
$$R_s = \alpha_s\, S_g\big|_{surface}$$

SPE-5

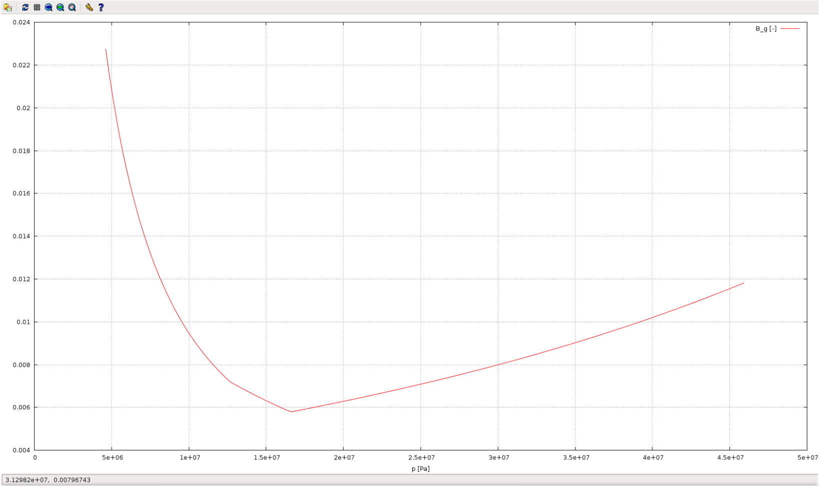
Thermodynamic parameters used to produce the results:

- 6 hydrocarbon components (C_1, C_3, C_6,C_{10}, C_{15}, C_{20})
- 2 phases (oil, gas)
- Isothermal ($T = 20^\circ C$)
- Initial reservoir pressure: 4 000 *PSI* (27.58 *MPa*)
- Initial oil composition:
  50% C_1, 3% C_3, 7% C_6, 20% C_{10}, 15% C_{15}, 5% C_{20},
- Cubic EOS (Peng-Robinson) for oil and gas phase
  - Non-linear densities, fugacity coefficients

Gas Formation Factor R_s



Gas Formation Volume Factor B_g



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3.12982e+07,  0.00796743
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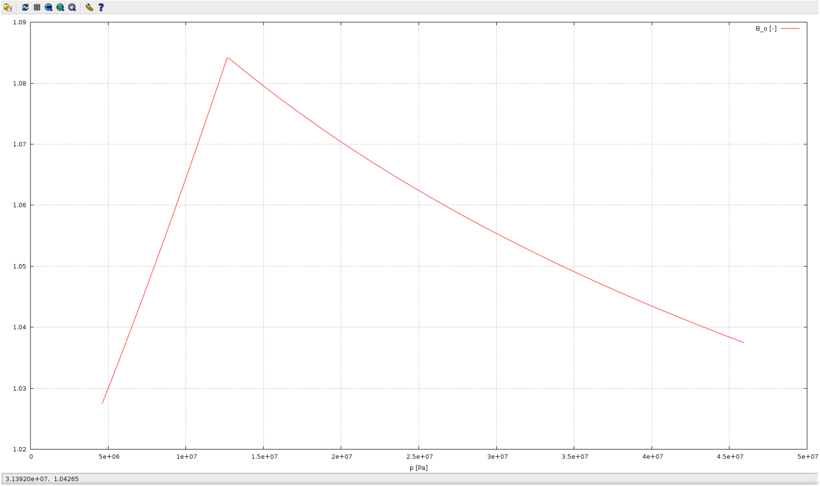
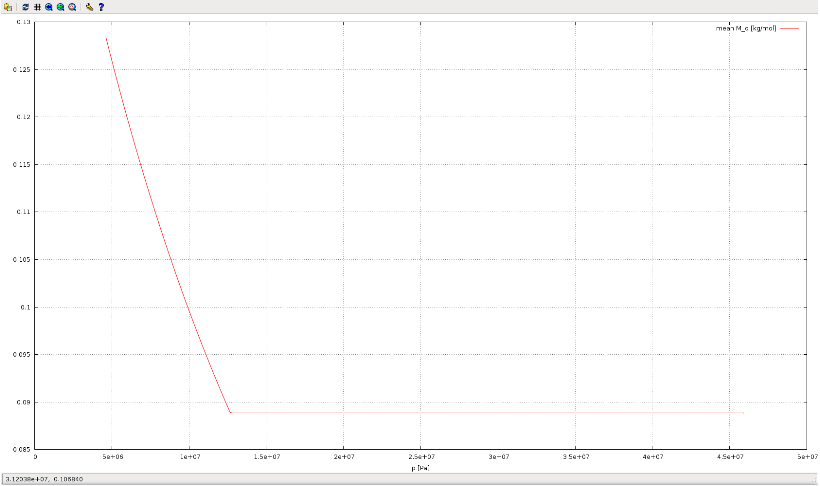
Gas Formation Volume Factor B_o

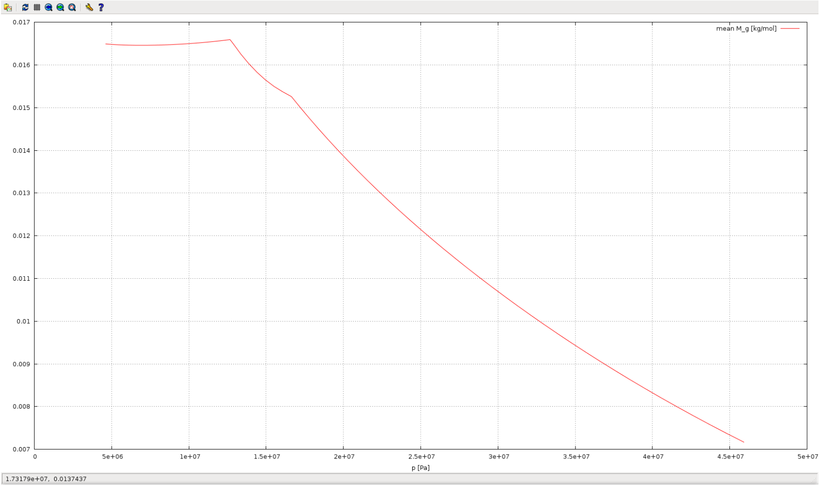


Mean Molar Mass of Reservoir Oil $\overline{M}_o$



3.12038e+07, 0.106840

Mean Molar Mass of Reservoir Gas $\overline{M}_g$



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