Four-phase equilibrium calculation algorithm for water/hydrocarbon mixtures

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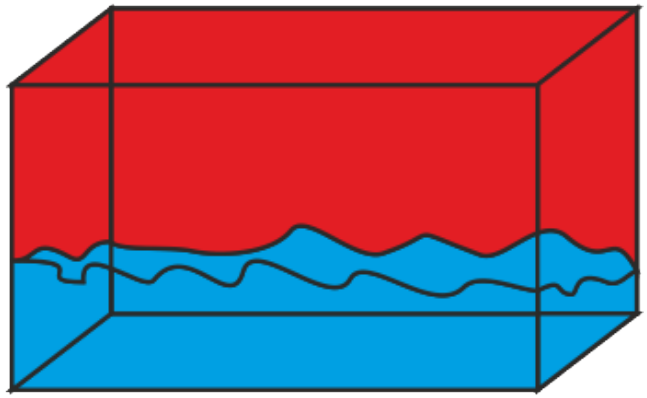
Motivation

- Phase-split calculations in 3, 4, and higher number of phases have broad applications.
- One major application is in compositional reservoir simulations.
- In a very large oil field, four different hydrocarbon phases have been observed: 2-liquid phases, a gas phase, and an asphaltene phase.
- Efficient and robust multiphase-split calculations have been a challenge until recently.
- Most of the mathematical procedures cover a limited range of conditions. We are interested in covering a very broad range of conditions.

Objective

- In phase split computations, our main objective is to cover a broad range of conditions to allow conditions in reservoir pressure and temperature, CO_2 injection, and separators.
- Two essential steps of phase-split computations are:
- Examination of stability
- Phase-split computations

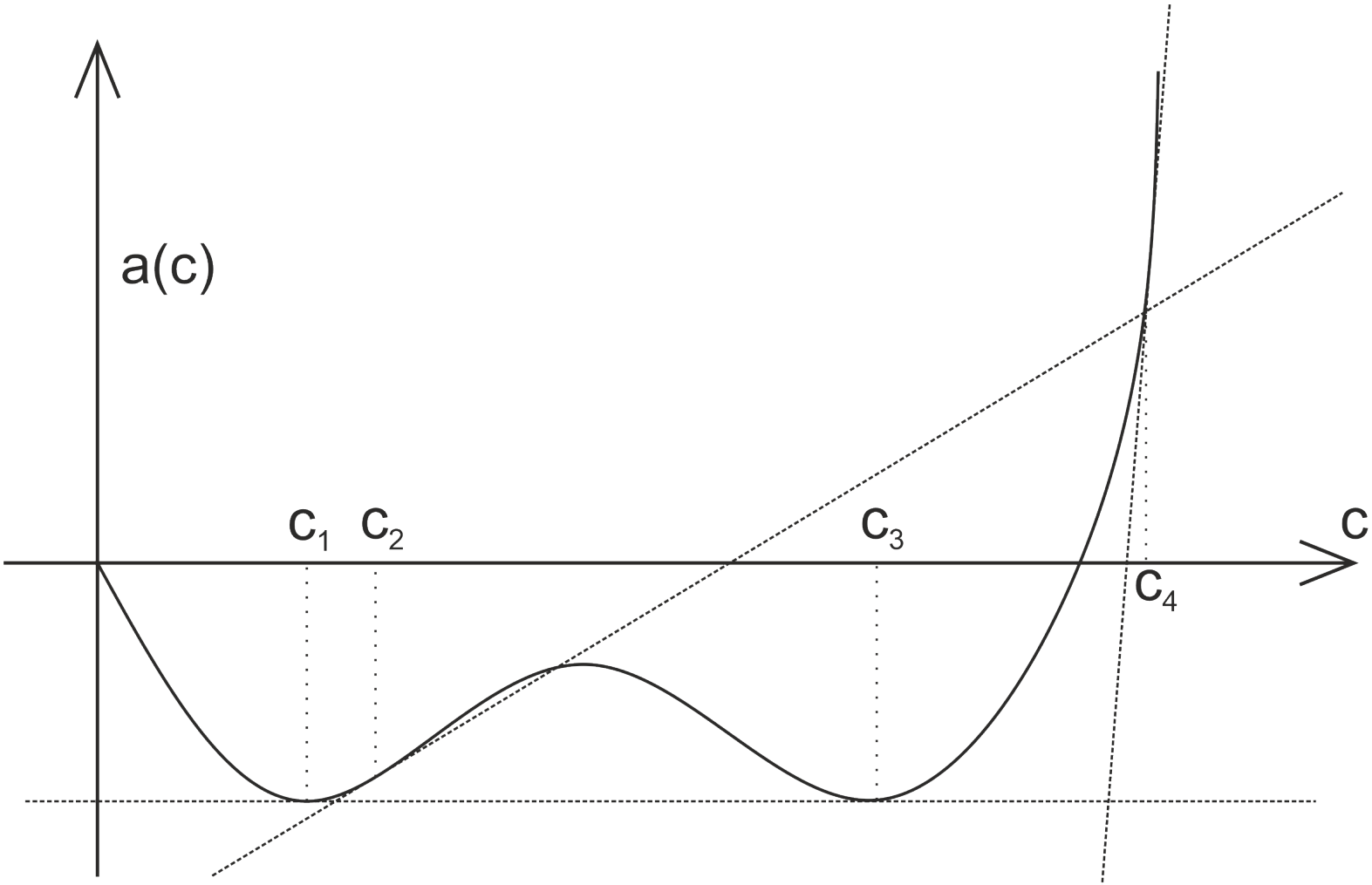


Stability

- First step is to examine stability of a phase (L. Michelsen 1982).
- Stability is done via TPD function, $TPD(\mathbf{x}^{trial}, \mathbf{x}^{test})$
- TPD function always has 1 trivial minimum with 0 value.
- A negative value of TPD implies phase instability.
- Global approach which is slow.
- Faster approach is to use local solvers which are fast but are in need of multiple initial guesses.
- $\mathbf{x}^{trial}$ with the negative TPD is then used as an initial approximation in phase-split calculations.

TPD function

- Three possible outcomes: stable, unstable, energically equivalent
- $a(c)$ is Helmholtz free energy density (VTN variables), same principles still hold.



Phase-split calculations

- A system of $n(c+1)$ equations for $n(c+1)$ unknows
- Equality of chemical potentials or fugacity coefficients

$$f_i^1(T, P, \mathbf{x}_1) = ... = f_i^n(T, P, \mathbf{x}_n), \quad i = 1, ..., c$$

- Material balance for components

$$z_i = \beta_1 x_{i1} + ... + \beta_n x_{in}, \quad i = 1, ..., c$$

- Mole fraction constraints

$$\sum_{i=1}^{c} x_{ij} = 1, \quad j = 1, ..., n$$

- The system of equation is solved by combination of succesive substitution technique (SSI) and Newton Rapson (NR).
- Symbols : n number of phases, c number of components in the mixture, f_i^j fugacity of component i and phase j

RR equation solution

- Solving the system of RR equations

$$f_j(\boldsymbol{\beta}) = \frac{\sum_{i=1}^{c}(1 - K_{ij})z_i}{1 - \left(\sum_{j=1}^{n-1}[1 - K_{ij}]\beta_j\right)} = 0, \quad j = 1, ..., n-1$$

- Problem is solved by Bisection in 2 phase (Mikyska 2023) and by NR with line search in 3 and 4 phases (Okuno 2010).
- is equivalent to solving the minimizations of the following function.

$$F(\boldsymbol{\beta}) = \sum_{i=1}^{c}\left(-z_i \ln\left|1 - \sum_{j=1}^{n-1}[1 - K_{ij}]\beta_j\right|\right)$$

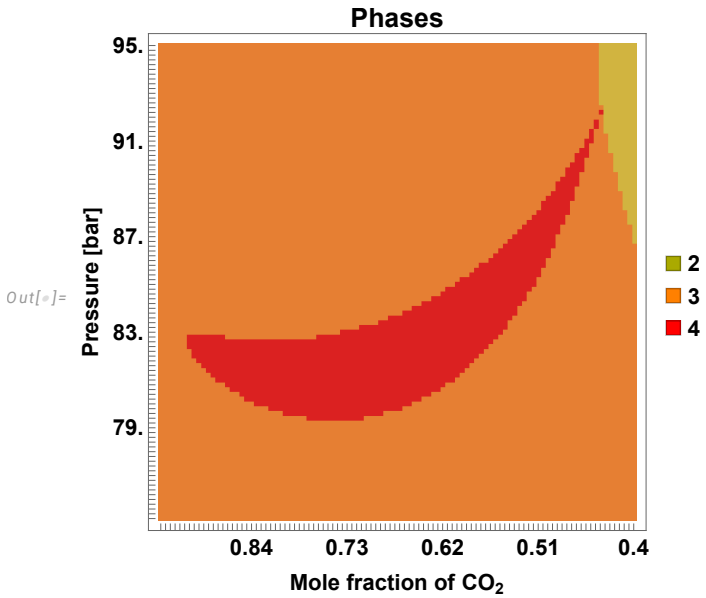
SSI

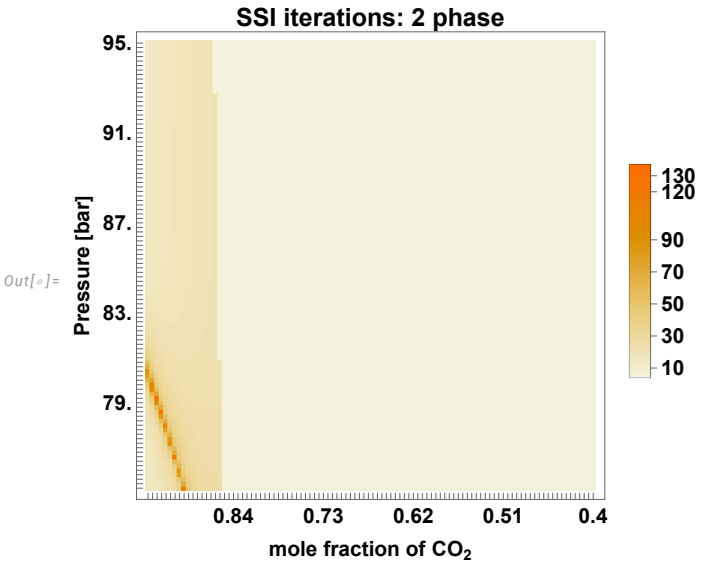
- 1. Solve RR equations, i.e. solve for β.
- 2. Calculate mole fractions $\mathbf{x}_j$ and compresibility factors from EOS.
- 3. Calculate fugacities f_i^j.
- 4. Update equilibrium ratios $K_{ij}^{new} = K_{ij}^{old} \exp[-\ln(f_i^j / f_i^n)]$.
- 5. Test the convergence, if close to solution switch to NR.

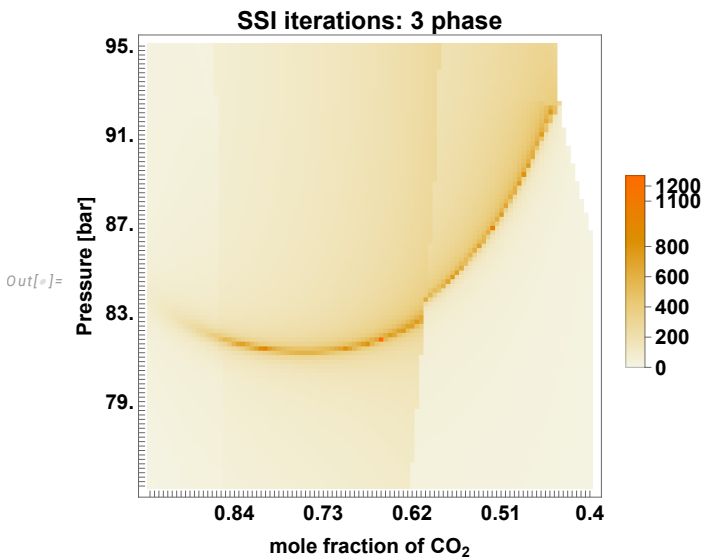
3 Examples -I. II.

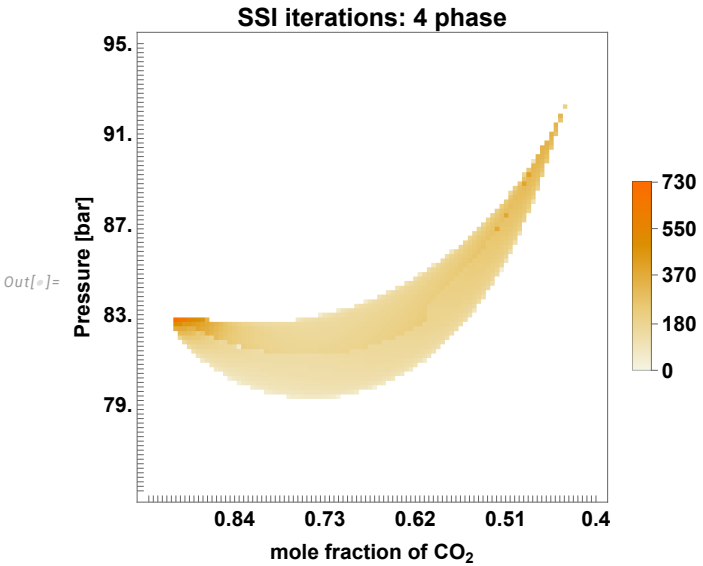
- Example I. 8 component mixture $[H_2O, C_1, C_{2-3}, C_{4-6}, C_{7-15}, C_{16-27}, C_{28+}, CO_2,]$ cP space,$75 - 95[bar]$, $40 - 100[\%]$ injection of CO_2 and $T = 313.71[K]$ (Imai et al. 2019)
- Example II. 7 component mixture $[CO_2, C_1, C_{2-3}, C_{4-6}, C_{7-14}, C_{15-25}, C_{26+}]$ cP space,$40 - 180[bar]$, $0 - 100[\%]$ injection of impure CO_2 and $T = 301.48[K]$ (Chen et al. 2023)

Example I. - Phase space and SSI iterations









Example II. - Phase space and SSI iterations

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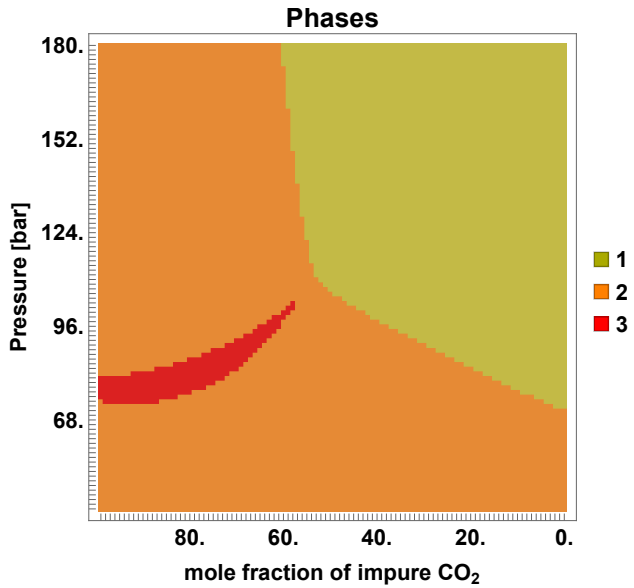

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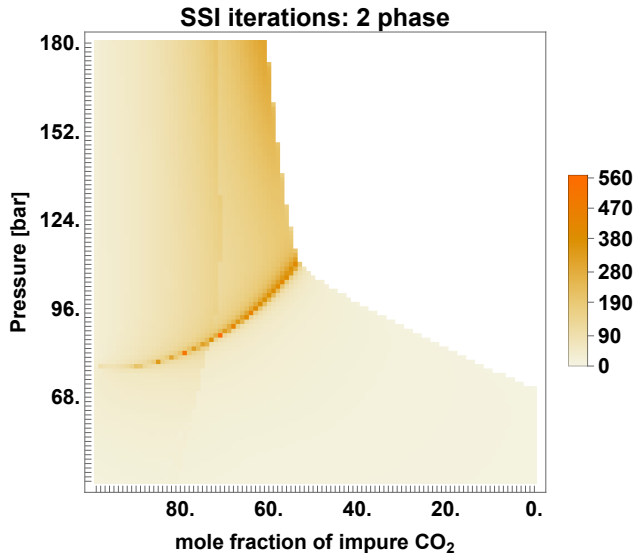

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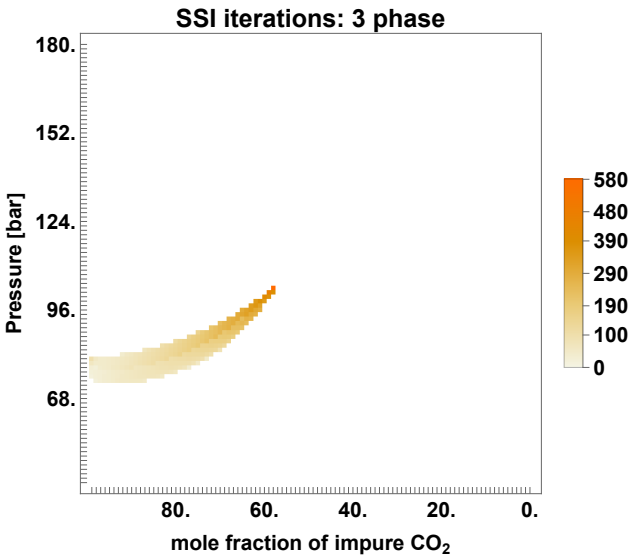

Concluding remarks

- The NR converges in less than two iterations in our implementation of phase-split computations except in some isolated spots.
- The SSI method has also high iterations in some regions.
- Our algorithm is fully robust in a wide range of conditions. We have examined ten different fluids which are considered complex by the authors in the literature. 300,000 independent calculations have been performed robustly.

Thank you for your attention!

- I am looking forward to your questions and comments.