Compositional simulation in OPM Flow: status and the way forward

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New Climit project!

- **Simulation tools for CO2 storage in depleted hydrocarbon fields - Phase 1 (SIMCO2DEPL)**
  - NORCE, SINTEF, EQUINOR and TNO.

- Development of a compositional field-scale simulator in OPM flow as one of the focus
  - Industrial setting

Existing prototype compositional simulator (developed in HPCG Climit project)

- Isothermal flash calculation (PT-Flash)
- Flow equations
  - Pressure, mole fractions, water saturation as primary variables
- Simple well model
  - Single connection with RATE and BHP control
- Input and output
- Tested with simple case

Compositional flow equations (oil-gas)

- For an oil-gas two phase system with N_c components, for each component *c*, the mass conservation equation is

$$\frac{\partial}{\partial t}\left(\phi\left(S_o\rho_o x_{oc} + S_g\rho_g x_{gc}\right)\right) + \nabla\cdot\left(\rho_o x_{oc}\mathbf{v}_o + \rho_g x_{gc}\mathbf{v}_g\right) = q_c$$

  - x_{oc} anc x_{gc} are the mass fractions of component *c* in oil and gas phase

$$S_o + S_g = 1$$

$$\sum_{c=1}^{N_c} x_{oc} = 1 \qquad \sum_{c=1}^{N_c} x_{gc} = 1$$

When water phase is involved

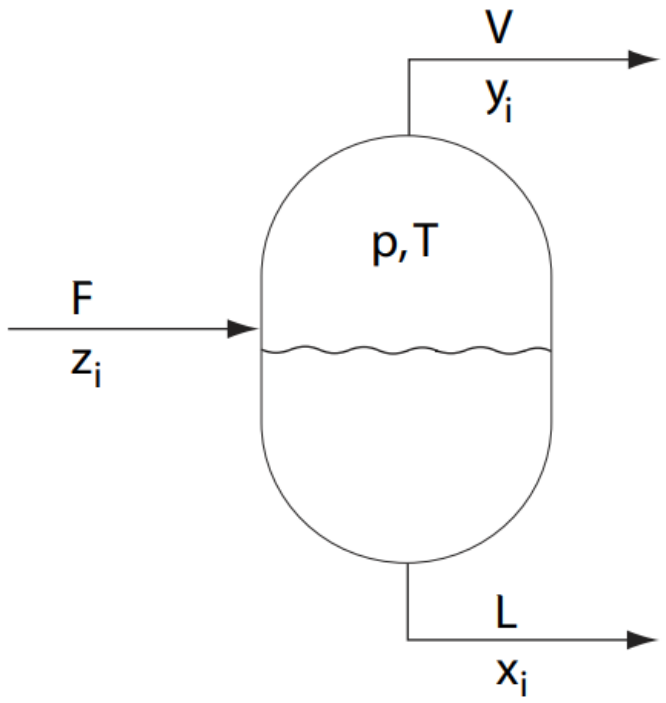
- Water is currently treated as an immiscible phase
  - Not involved in the flash calculation
  - Will be extended to be miscible in the late development

$$\frac{\partial}{\partial t}\left(\phi S_w \rho_w\right) + \nabla \cdot \left(\rho_w \mathbf{v}_w\right) = q_w$$

$$S_o + S_g + S_w = 1$$

Isothermal flash calculation

- Given
  - Pressure *P* and Temperature *T*
  - Molar fractions of the component *c* z_c
- Determine
  - Liquid fraction *L*
  - Molar fractions for each phase x_c and y_c
  - Saturations and phase properties
    - density, viscosity and so on
- Used in
  - Flow modeling
  - Surface separation (well modeling)



https://skoge.folk.ntnu.no/bok/mer/flash_english_edition_2009

Isothermal flash calculation (continued)

- Different equations of states can be used
  - Peng-Robinson (PR), Corrected Peng-Robinson (PRCORR), Redlich-Kwong (RK), and Soave-Redlich-Kwong (SRK)

- Solution techniques
  - Successive substitution iteration (SSI), Newton method and Hybrid SSI-Newton

- Implicit differentiation is used to get derivatives after flash calculation

$$\mathbf{G}\left(\eta, \boldsymbol{\beta}(\eta)\right) = 0 \rightarrow \frac{d\mathbf{G}}{d\eta} = \frac{\partial \mathbf{G}}{\partial \eta} + \frac{\partial \mathbf{G}}{\partial \boldsymbol{\beta}} \frac{\partial \boldsymbol{\beta}}{\partial \eta} = 0 \rightarrow \frac{\partial \boldsymbol{\beta}}{\partial \eta} = -\left(\frac{\partial \mathbf{G}}{\partial \boldsymbol{\beta}}\right)^{-1} \frac{\partial \mathbf{G}}{\partial \eta}$$

Møyner O. Compositional Simulation with the AD-OO Framework. In: Lie K-A, Møyner O, eds. *Advanced Modeling with the MATLAB Reservoir Simulation Toolbox*. Cambridge University Press; 2021:324-374.

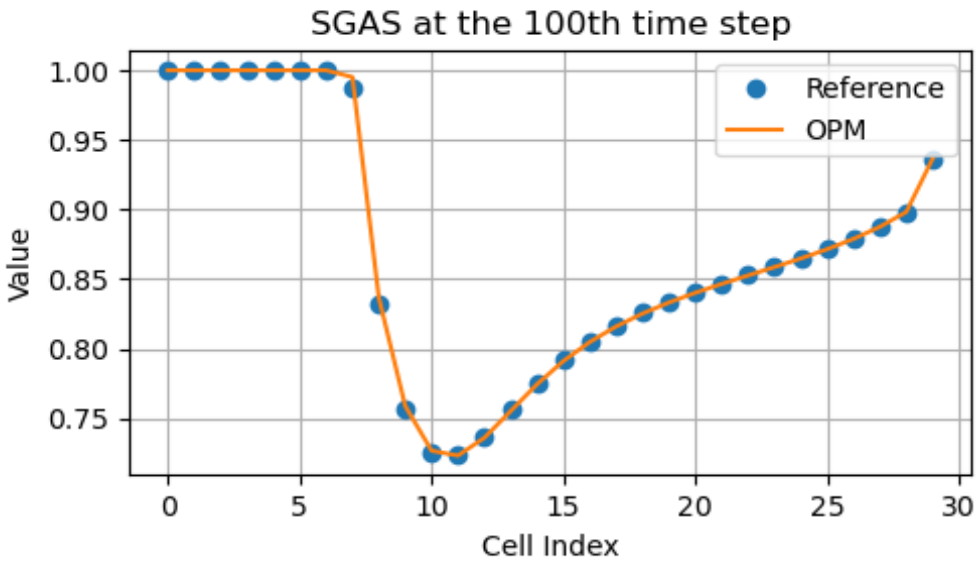
A simple well model (single connection)

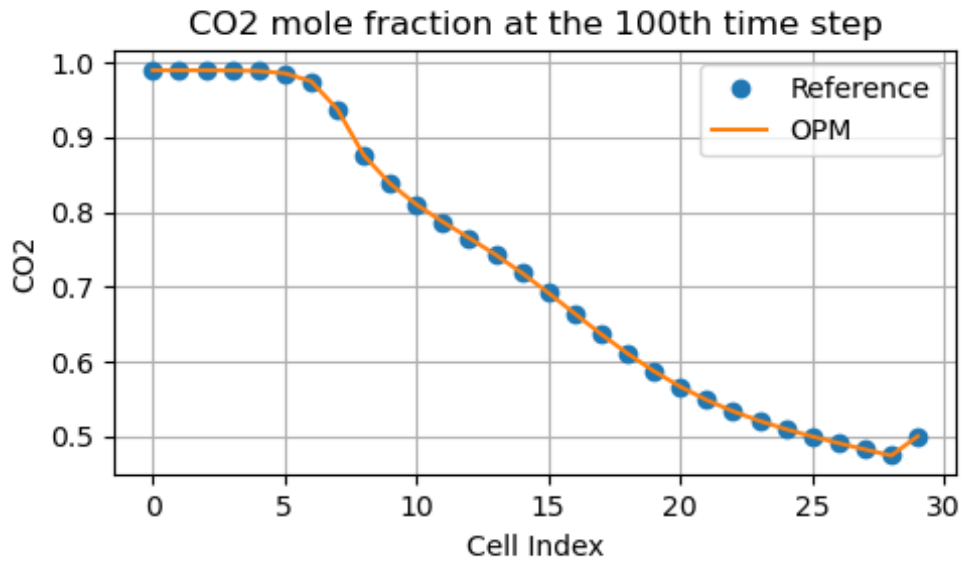
- Mass conservation equations for N_c components

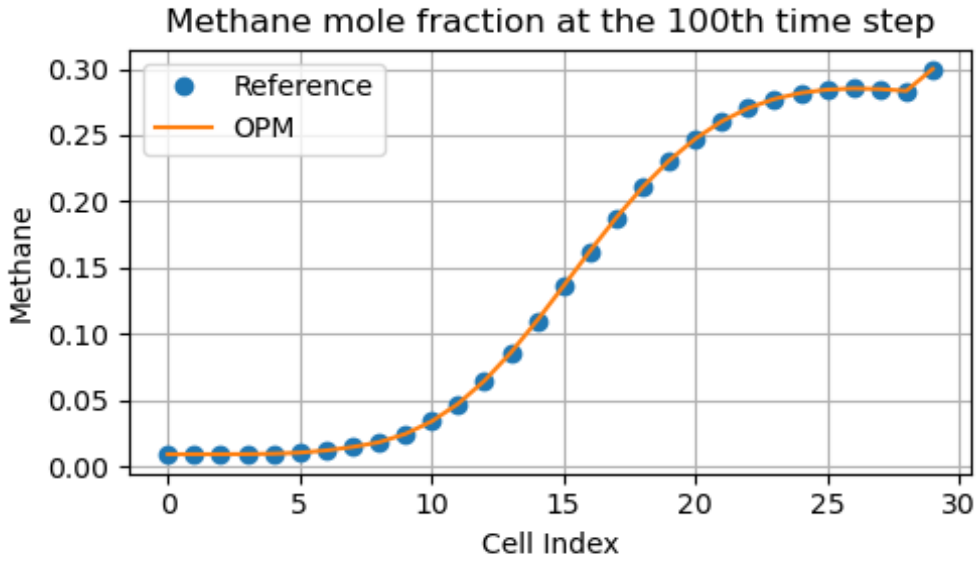
$$\frac{d}{dt}(M_c) + \sum_{perf=1}^{N_{perf}} q_c - Q_c = 0$$

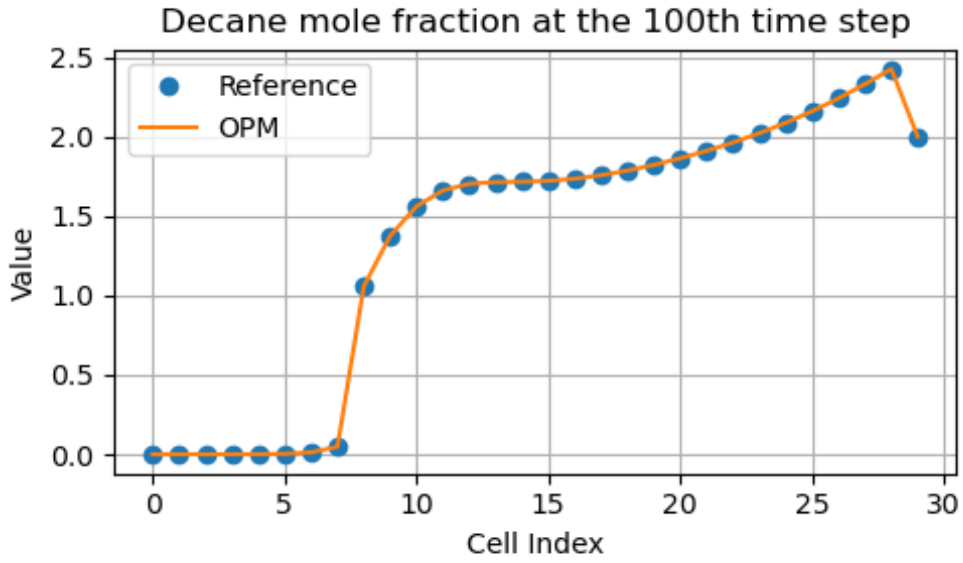
  - q_c is the mass rate for component *c* for *perf*
  - Q_c is the injection/production mass rate for component *c*
  - M_c is the mass of component *c* in the wellbore
- Well control equations
  - BHP control $P_{bhp} - P_{bhp}^{target} = 0$
  - RATE control for phase *p* $Q_p - Q_p^{target} = 0$

Validation against reference result (oil-gas)

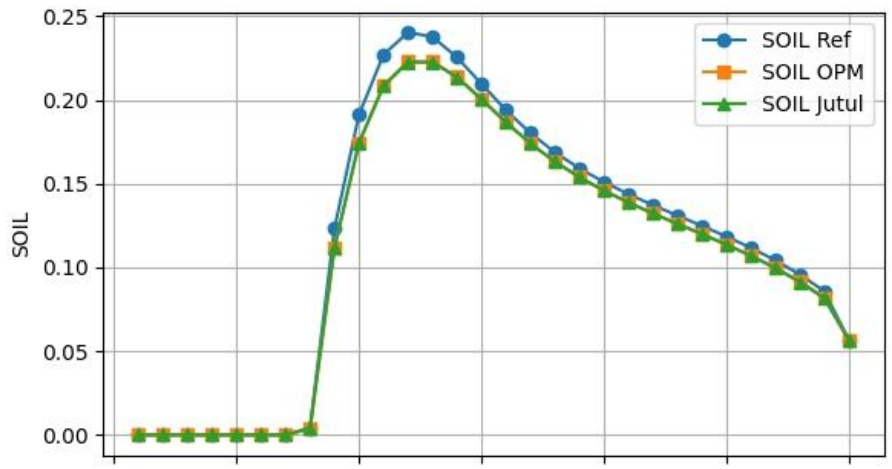


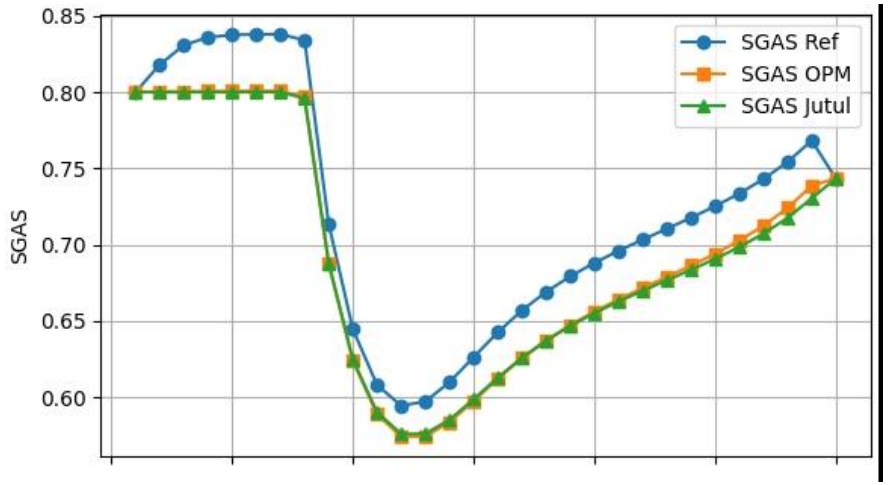


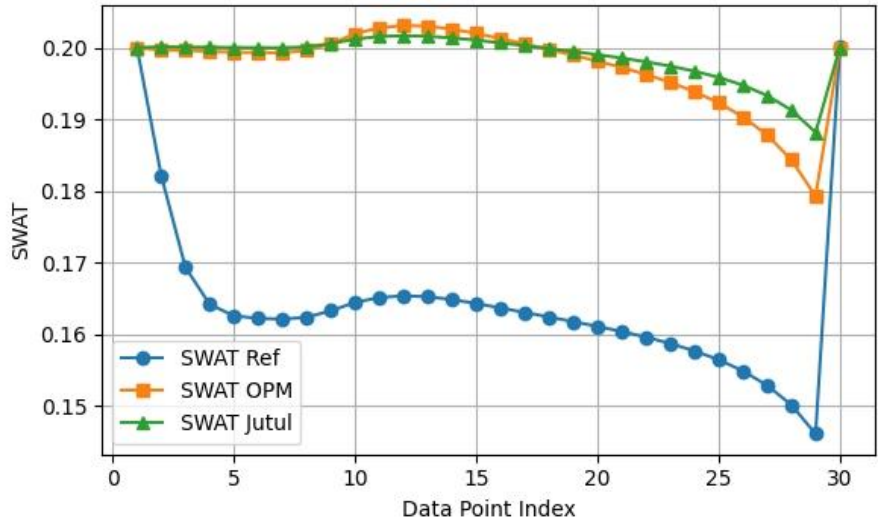




Validation against reference result (with water)

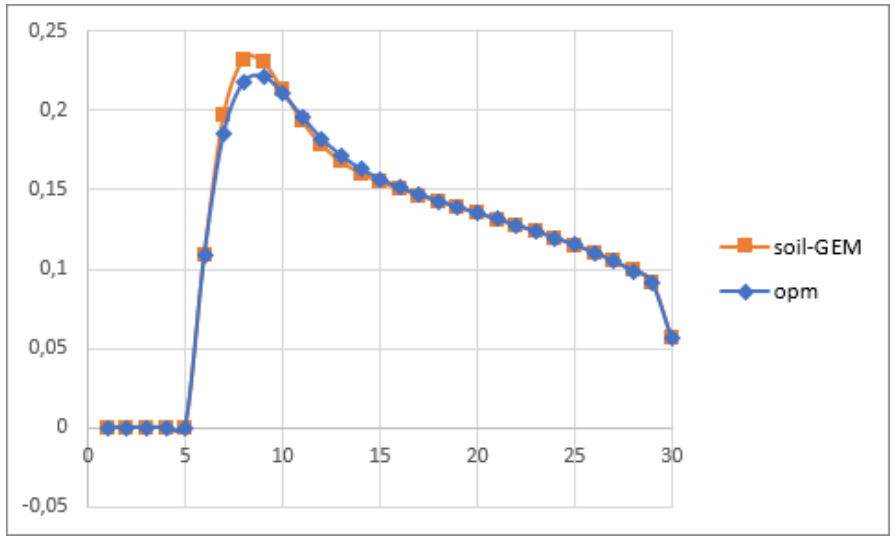


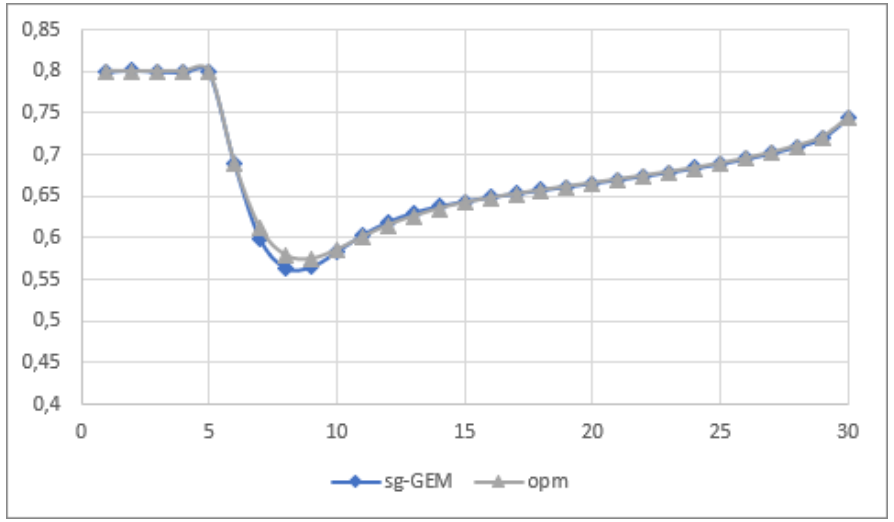


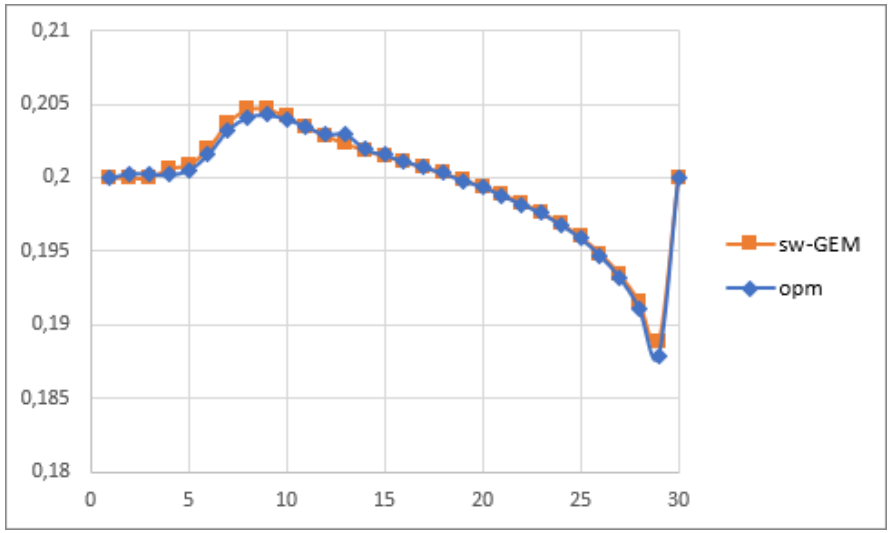


Different way of initializing saturations are seen against the reference simulator

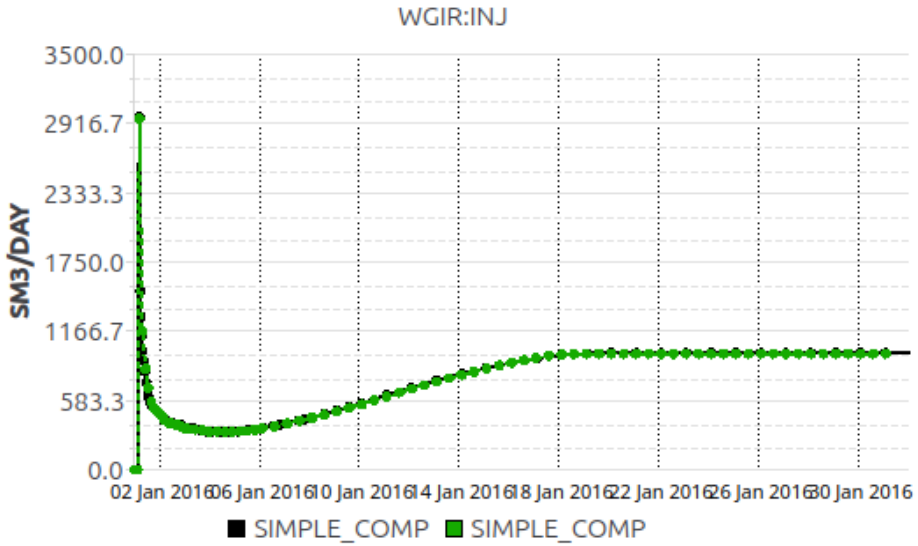
Validation against GEM (with water)

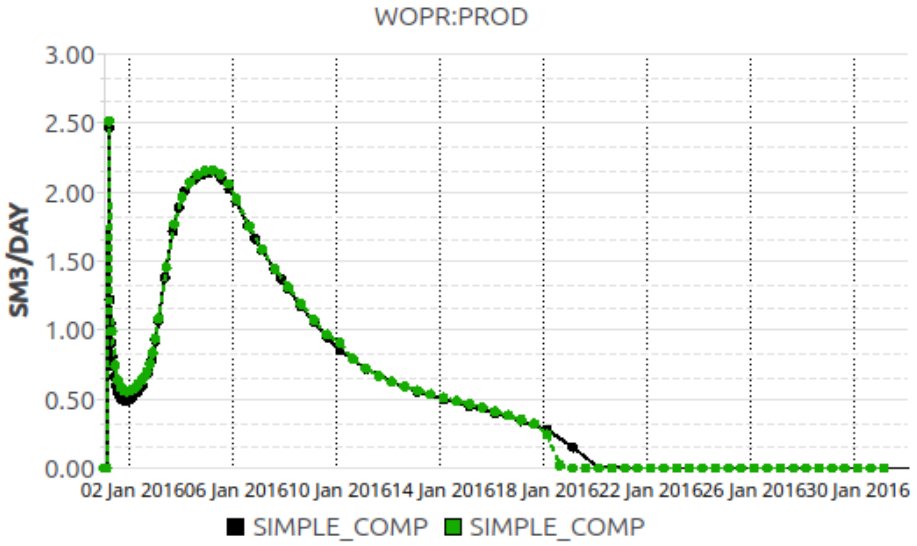


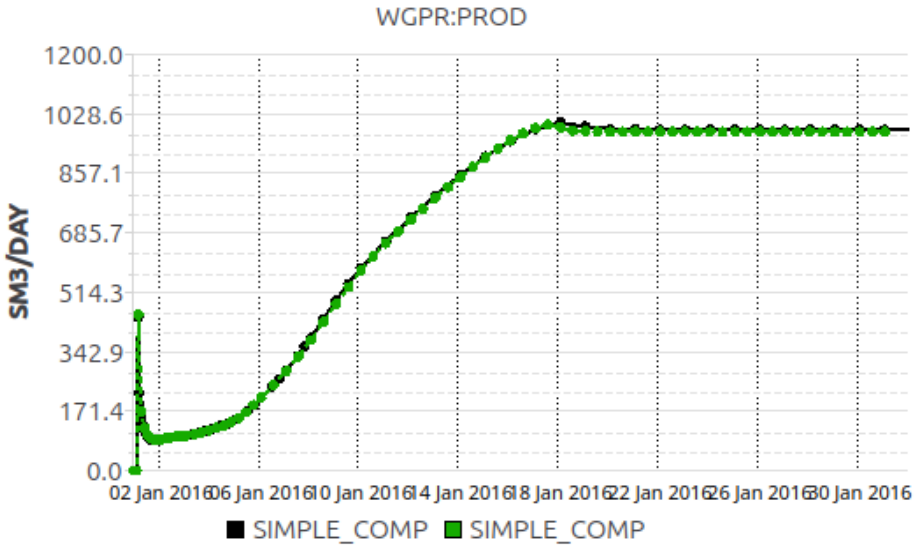




Simple well model







The way forward

- Further develop the existing prototype to simulate realistic field models.
- Simulate the production/depletion of hydrocarbon fields before the CO2 injection start (historical period)
- Simulate the CO2 injection in a realistic prediction setup
- Many important functionalities are missing from the existing prototype compositional simulator

The way forward (cont'd)

- Equilibration (to be discussed later)

- Well modeling
  - Standard wells with multiple connections
  - Multisegment wells
  - Various rate control, BHP and THP control

- Group control and network modeling
  - Prediction
  - It is possible to test different strategies to improve current OPM-flow group control and network modeling facilities

The way forward (cont'd)

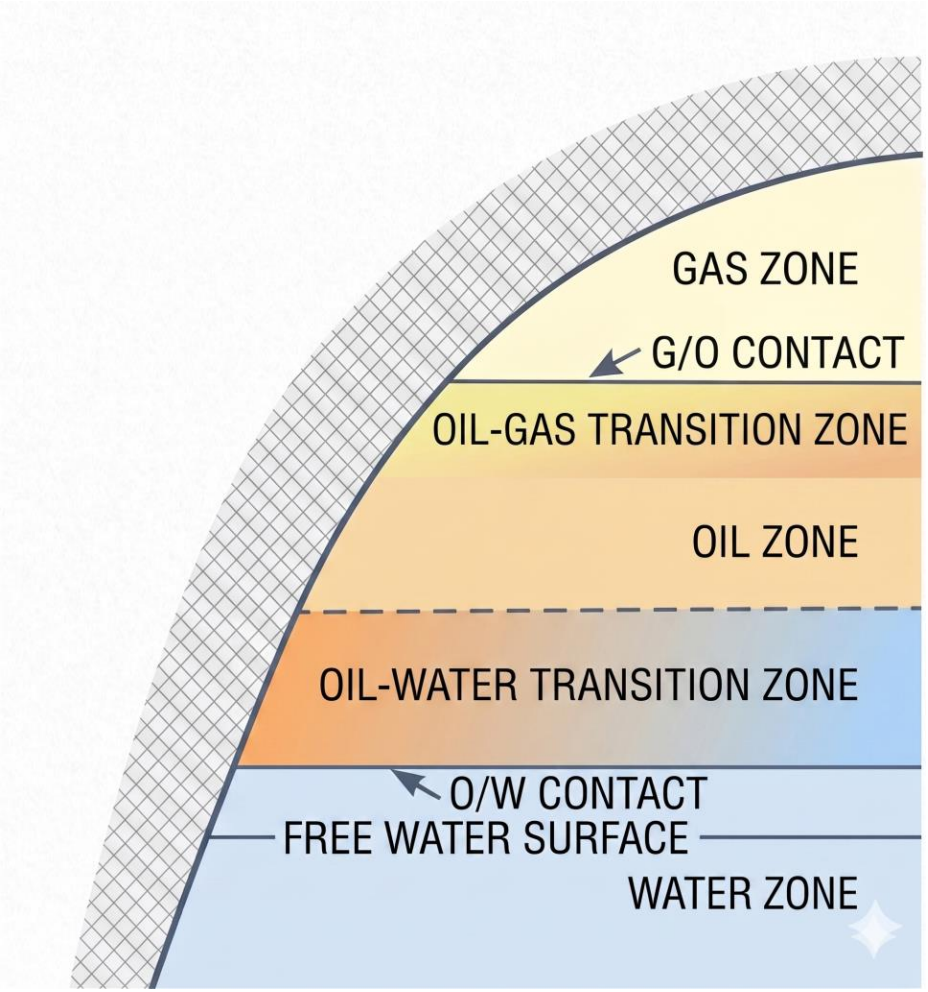
- Thermal simulation that the temperature of the field can be dynamically changed
  - PT-Flash be extended to handle the derivative of the temperature (**done**)
  - Temperature will be a new primary variable (WIP)
  - Energy conservation based internal energy and enthalpy (WIP)
  - Energy equation for the wells

- Enthalpy based thermal modeling (prototype)
  - Enthalpy is a primary variable (instead of temperature)
  - Pressure-Enthalpy (PE) Flash calculation
  - More robust for phase transition
  - Simulation with pressure and temperature near critical points will be tested

Way forward (cont'd)

- Performance and robustness
  - Linear solver and non-linear solution technique
    - CPRW
  - Parallel simulation
  - Time stepping
  - Moving from the current experimental framework to Flow
- Industrial level input and output facility
- Testing with realistic field setting

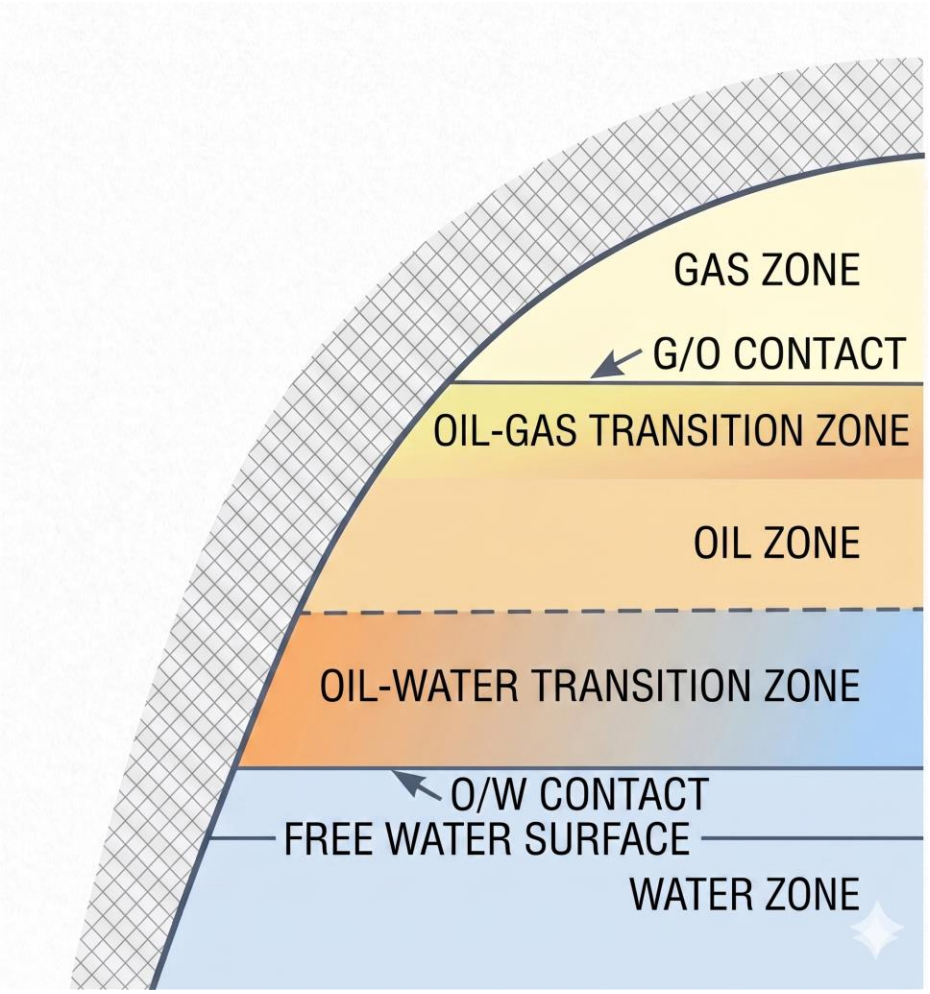
Compositional Equilibration (WIP)



Accurate equilibration is the foundation of realistic reservoir simulation. It ensures that the numerical model starts in a state of quiescence (no flow), where pressure, saturation, and fluid compositions are balanced according to geological, capillary, and thermodynamic forces.

Without this, the simulator will produce artificial, spurious flows in the first few timesteps, leading to inaccurate forecasting and history matching.

Equilibration in the black oil setting




```
EQUIL
-- Datum     P       woc      Pc     goc       Pc   Rsvd  Rvvd
 2561.59   268.55  2645.21   0.0   2561.59   0.0    1      0    0 /

RSVD
 2561.59   122.30
 2697.0    106.77 /
```

- Datum depth and datum pressure
- Gas-oil-contact depth, and capillary pressure at the depth
- Water-oil-contact depth, and capillary pressure at the depth
- Rs value changing with the depth
- Rv can also be specified

Equilibration in the black oil setting (cont'd)

Pressure

$$P_o(Z) = P_{datum} + \int_{Z_{datum}}^{Z} \rho_o(P) \cdot g \, dZ$$

$$P_g(Z_{GOC}) = P_o(Z_{GOC}) + P_{cog}|_{GOC}$$

$$P_g(Z) = P_g(Z_{GOC}) + \int_{Z_{GOC}}^{Z} \rho_g(P) \cdot g \, dZ$$

$$P_w(Z_{WOC}) = P_o(Z_{WOC}) - P_{cow}|_{WOC}$$

$$P_w(Z) = P_w(Z_{WOC}) + \int_{Z_{WOC}}^{Z} \rho_w(P) \cdot g \, dZ$$

Saturation

$$S_w(Z) = P_{cow}^{-1}(P_o - P_w)$$

$$S_g(Z) = P_{cog}^{-1}(P_g - P_o)$$

$$S_o(Z) = 1 - S_w - S_g$$

Equilibration with compositional (WIP)

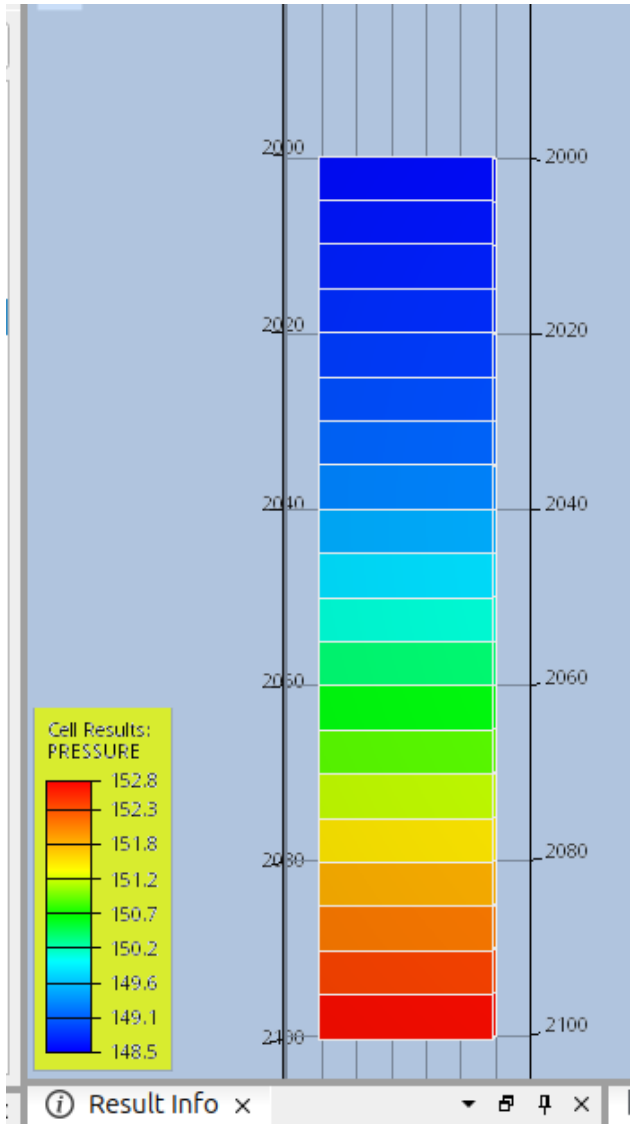
```
EQUIL
-- datum  datum   WOC    WOC    GOC    GOC              Type Set_SAT
-- depth  press   depth  Pcow   depth  Pcog
   2010     150    2300   0      2050     0   2* 1*     1    1* /
```

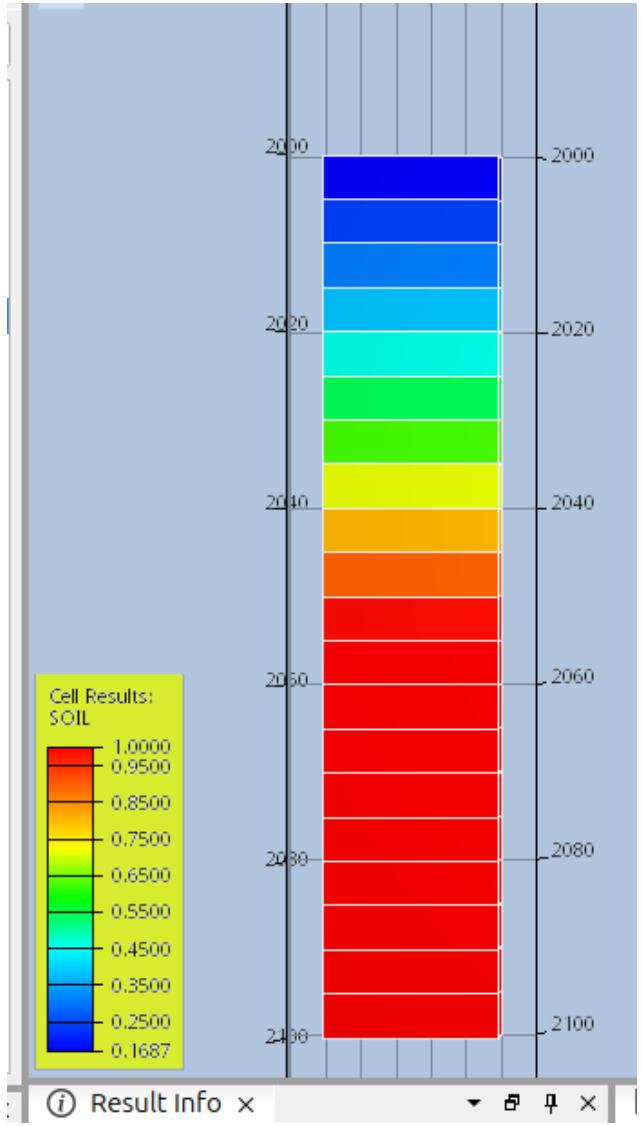
```
ZMFVD
-- depth  CO2  METHANE DECANE
   2000   0     0.7     0.3
   2100   0     0.3     0.7  /
```

- Datum depth and datum pressure
- Gas-oil-contact depth, and capillary pressure at the depth
- Water-oil-contact depth, and capillary pressure at the depth
- **ZMFVD to specify mole fractions for the components along depth**

Equilibration with compositional (first shot)

- We use the same calculation procedure, while replace the black-oil PVT density calculation with PT-flash based density calculation





Equilibration with compositional (WIP)

- It **does not** run with the reference simulator
- Reference simulator question whether we set the composition at the GOC correctly, with item 10 to be 1 (continuous hydrocarbon initial state)
- It is basically saying that the setup for GOC depth is not physically viable or consistent

Equilibration with compositional (WIP)

```
EQUIL
-- datum   datum    WOC     WOC     GOC     GOC                  Type Set_SAT
-- depth   press    depth   Pcow    depth   Pcog
   2010      150     2300    0       2050      0    2* 1*         1     1* /
```

- Item 10 defines three types of initialization types for compositional
  1. Continuous hydrocarbon phase initial state (no gas-oil contact)
     - Maybe GOC depth should be removed, while is it desirable?
  2. Gas-oil contact, vapor composition at the contact. Pressure at the datum depth will be replaced by saturation pressure
  3. Gas-oil contact, liquid composition at the contact. Pressure at the datum depth will be replaced by saturation pressure

- Item 11, if set to be 1, with option 2 and 3, not replacing the pressure at the datum depth by saturation pressure

Equilibration with compositional (WIP)

- Guidelines/input from experienced reservoir engineers is required for further development
  - What is the practical and correct way to set up realistic reservoir with compositional setting.
  - How to manage the potential higher requirement of physical consistency.
  - If saturation is calculated from the capillary pressure, whether/how to make sure the saturation is consistent with the fluid composition, pressure, and temperature setting.

Summary

- The compositional simulator we have is still in the early stage, various improvements, big and small, will be needed to mature the simulator

- Hopefully, it will be relatively fast by incorporating existing development from black-oil simulator
  - Parsing, schedule, grid, parallelization, linear/nonlinear solvers, input/output facility, surface facility, time stepping, etc.

- We need to work closely with engineers that are experienced in compositional reservoir simulation and CCUS

Acknowledgement

- The work is done through the new SIMCO2DEPL project sponsored by GassNova and Equnior

- Looking forward to more rewarding collaborations coming, more reporting, discussion and sharing of the new development in the future events

Thank you!