Compositional Simulation Development in OPM-flow

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Background

- OPM-flow has been mostly a black-oil reservoir simulator
  - Three-phase flow, PVT for fluid property evaluation
  - Field-scale deployment, proven robustness

- Compositional simulation
  - Multi-component, Equations of state (EOS)-based
  - Gas injection and miscible displacement
  - More generic and potentially more accurate simulation for EOR/CCUS scenarios
  - Experimental work to further expand the simulation capabilities of OPM-flow
    - Based on the great work of OPM-flow

A brief (incomplete) history

- PT-Flash two phase calculation — June 2022
  - SSI, Newton, and SSI+Ne
  - Peng-Robinson (PR) equation of state
  - AD based, Implicit differentiation to get the derivatives after the flash calculation
- A pressure driven CO2 flooding 1D demonstration — Nov. 2023
- Extending fluid system to allow any number of components — Dec. 2023
  - Oil-Gas two phase
- Running simulation from DATA input file — Sep. 2024
  - Keywords parsing and utilizing in simulation
- Summary and Restart output — Oct. 2024
- Run DATA files with different number of components — Oct. 2024
- Extending the fluid system to incorporate an immiscible water phase — Nov. 2024
  - Oil-Gas-water
- More equations of states — Jan. 2025
  - PRCORR, RK and SRK
- A simple compositional well model — Feb. 2025
  - Single connection, oil-gas two phase, BHP and RATE control.

Compositional flow equations

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

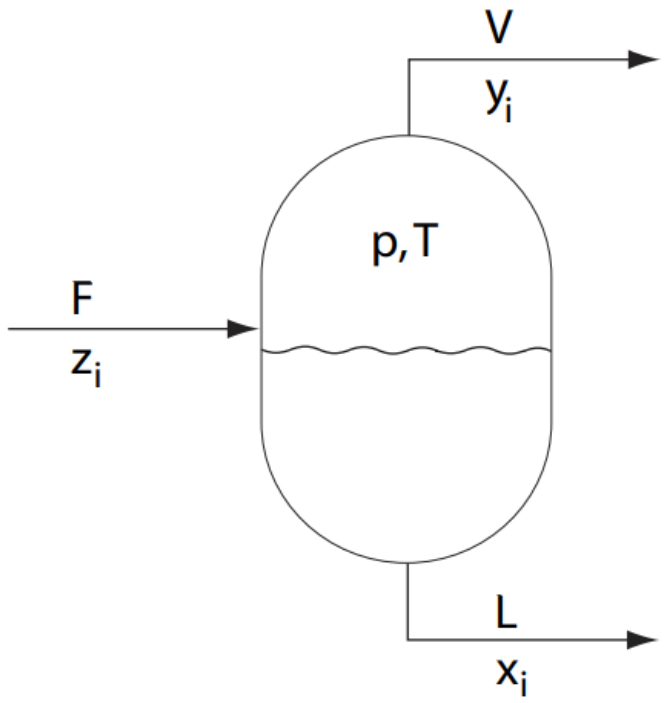
$$\frac{\partial}{\partial t}\left(\phi\left(S_o\rho_o x_{oc} + S_g\rho_g x_{gc}\right)\right) + \nabla\cdot\left(\rho_o x_{oc}\mathbf{v}_o + \rho_g x_{gc}\mathbf{v}_g\right) = q_c$$

  - ϕ : porosity
  - S_o, Sg : saturation for oil/gas phase
  - ρ_o, ρ_g : densities for oil/gas phase
  - x_{oc}, x_{gc} : mass fractions of component *c* in oil/gas phase
  - $\mathbf{v}_o, \mathbf{v}_g$: Darcy velocity for oil/gas phase

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

Isothermal flash calculation

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



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
  - Hybrid SSI-Newton

- Implicit differentiation is used to get derivatives after flash calculation

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

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.

When water phase is incorporated

- Water is currently treated as an immiscible phase
  - Not involved in the flash calculation
  - Can be changed/extended in a later stage

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

$$S_o + S_g + S_w = 1$$

Primary variables for the flow equations

- Pressure P
  - No capillary pressure
- Molar fractions for the $\{1..N_c\text{-}1\}$ components z_c
- Water saturation (if needed) S_w
- Temperature (if needed) T
  - Not implemented

Well modeling

- 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* $Q_p - Q_p^{target} = 0$

Primary variables for the well modeling

- Total surface rate Q_t
  - might switch to total mass rate
- Molar fractions for the $\{1..N_c\text{-}1\}$ components z_c
- Bottom hole pressure P_{bhp}

Surface separation process

- In the black-oil simulation, the surface densities is predefined
  - DENSITY

- In compositional simulation, a flash calculation is performed under **surface condition** to evaluate the surface fluid properties for oil and gas phase, so we can convert fluid quantities between reservoir condition and to surface condition
  - **surface phase densities**
  - **volume fractions (saturations)**
  - **mass fractions for each component**

- For the producers, the composition of the fluid from the wellbore is dynamic and the derivatives need to be considered.
  - By using AD, it has been relatively straightforward.

- The above represents single-stage separation process, can be extended to handle multi-stage separators

Supported compositional keywords

- COMPS
- EOS

- CNAMES, ACF, MW, PCRIT, TCRIT, VCRIT, BIC

- XMF, YMF, ZMF
- WINJGAS, WELLSTRE

They are used along with other many other existing keywords for compositional simulation

Demonstration

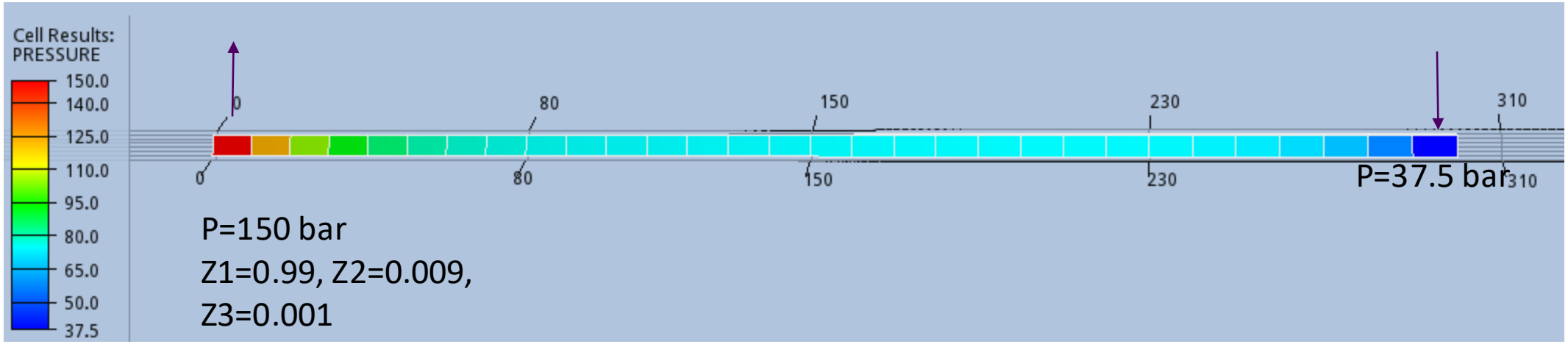
- flowexp_comp

- Some of the arguments:
  - --output-dir (output path)
  - --enable-vtk-output (false by default)
  - --flash-two-phase-method (ssi, newton and ssi+newton, ssi by default)
  - --flash-verbosity (0 by default)

- flowexp_comp 1D_COMP.DATA --output-dir=outputdir --enable-vtk-output=true

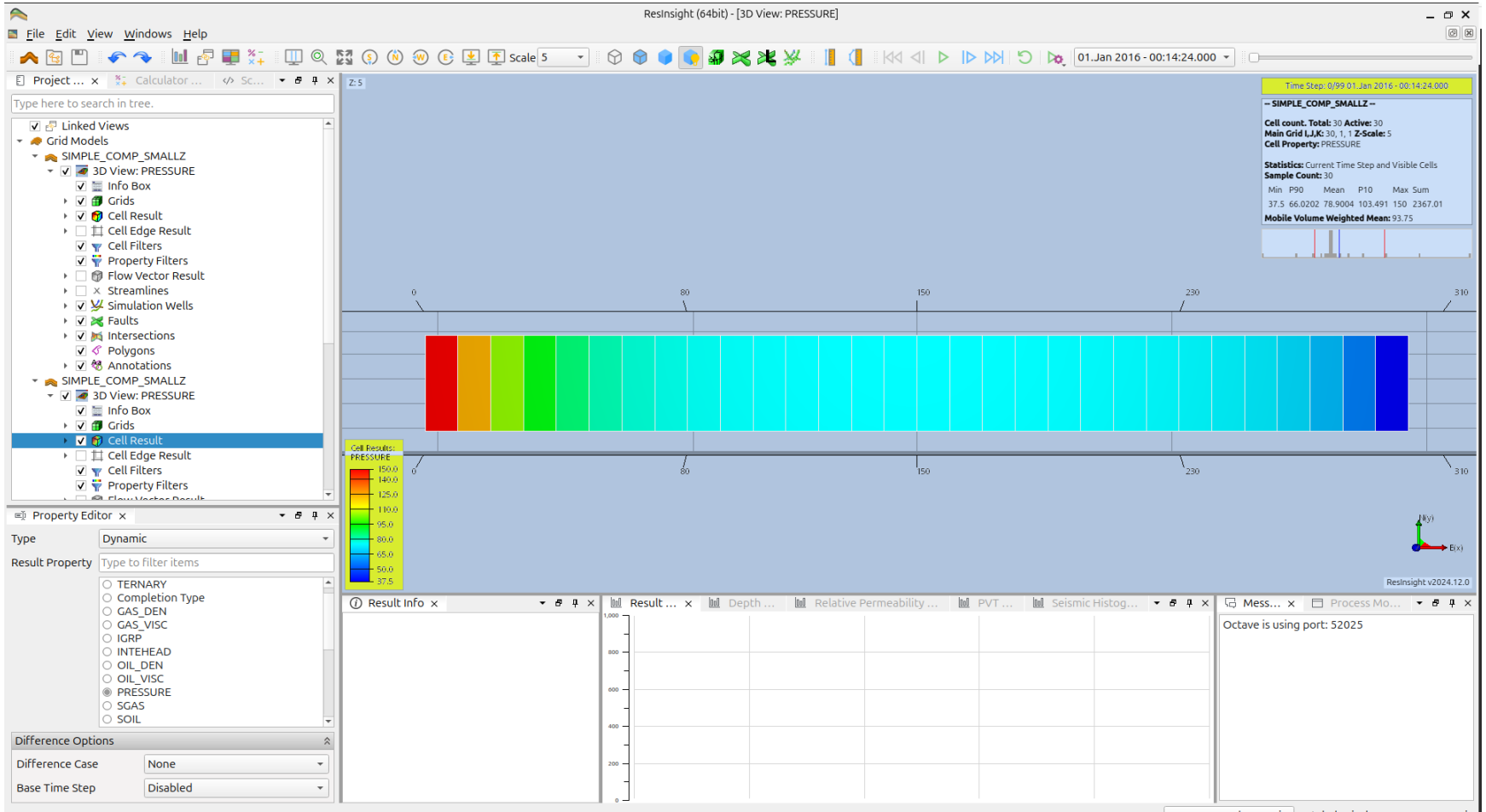
Test Case 1

- 1-D model (30x1x1), with two phase and three components
- K=100 mD, Phi=0.1, P_{res}=75 bar, S_{Gas}=1, T_{res}=150 °C,
- Components (CO2(1), CH4(2), Decane(3)), Z_1=0.5, Z_2=0.3, Z_3=0.2
- Cell(1,1,1) and cell(30,1,1) are assigned with much bigger pore volume to mimic source and sink with constant pressure and compositions

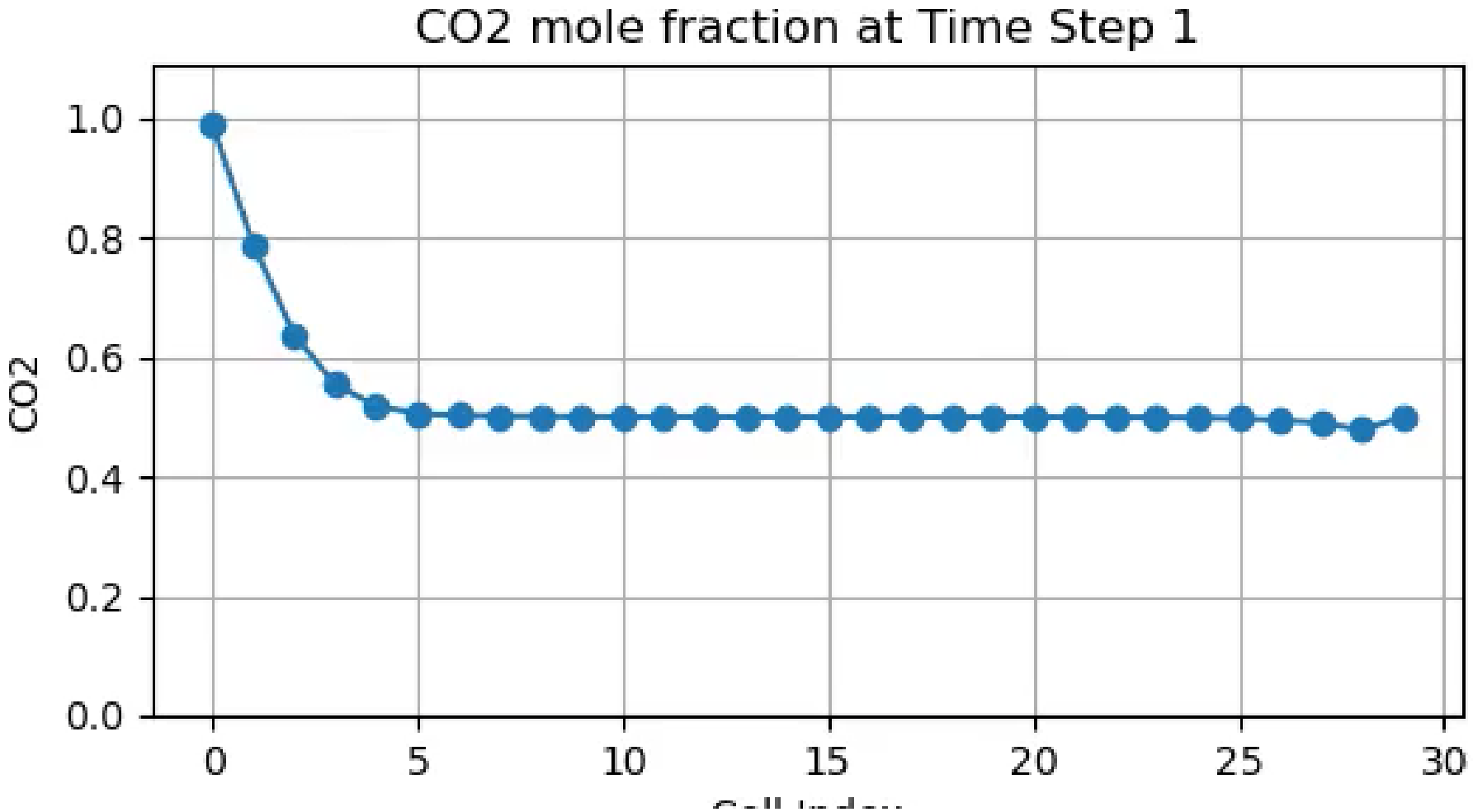


Visualization

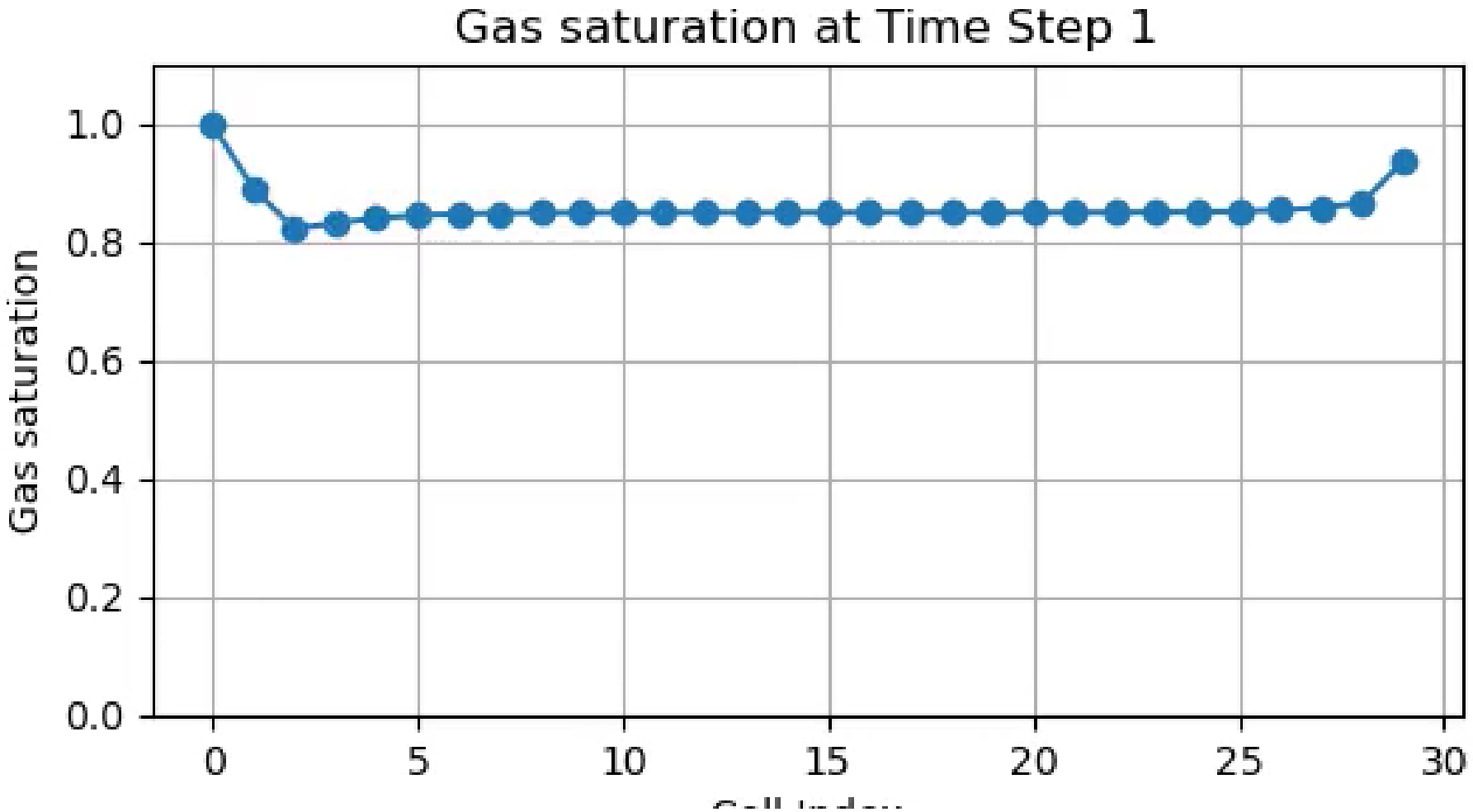
- Both VTK and UNRST output is supported and can be visualize with ResInsight and Paraview



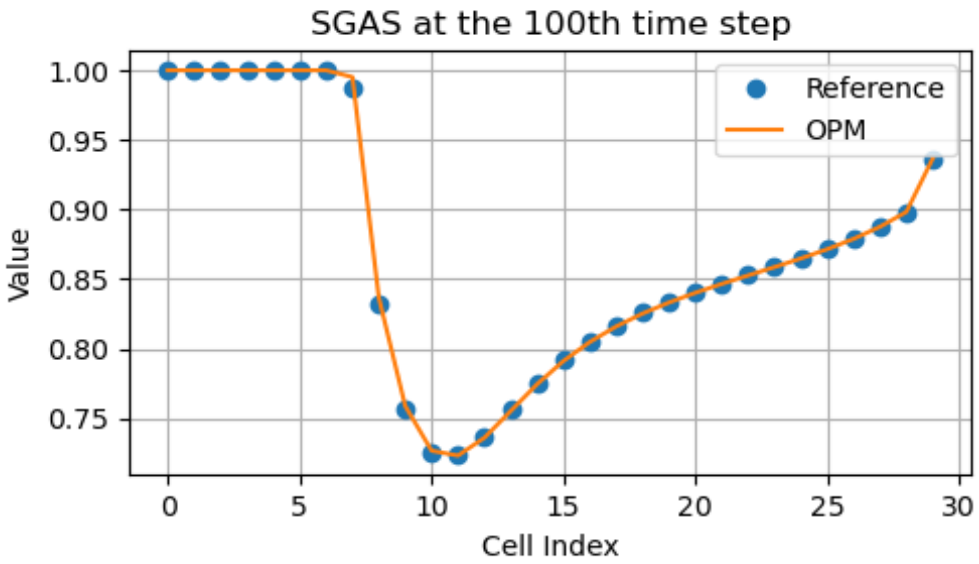
Resulting CO2 mole fraction evolution against reference result

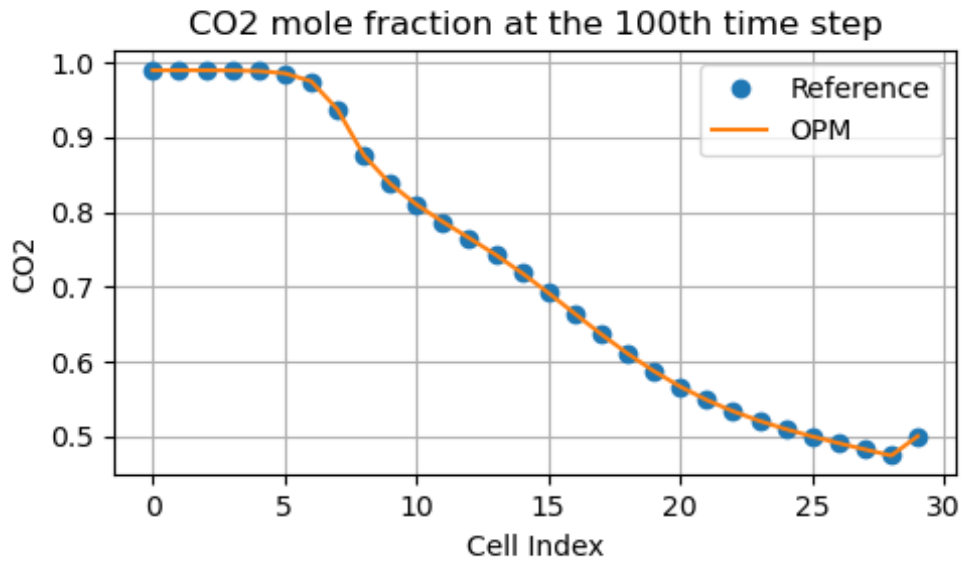


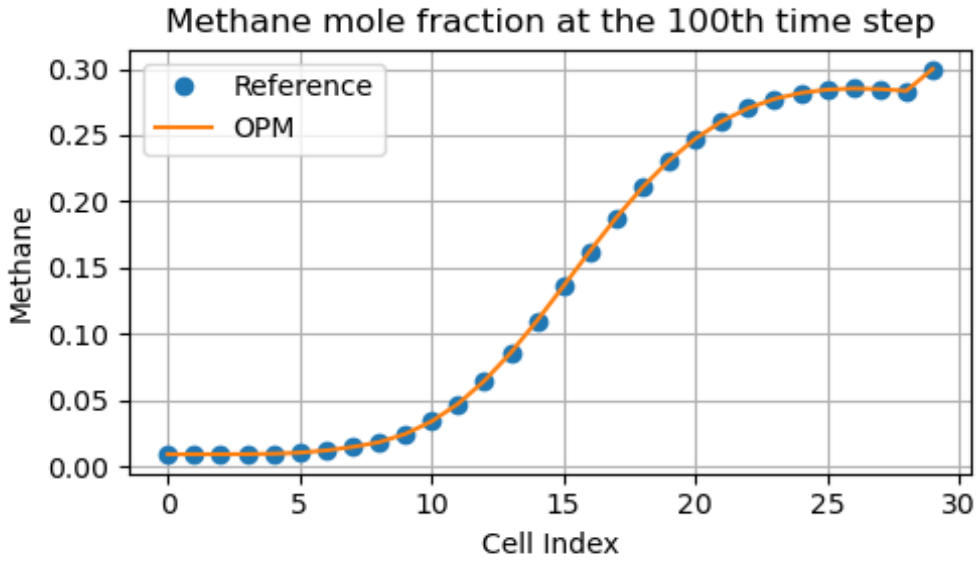
Resulting gas saturation evolution against reference result

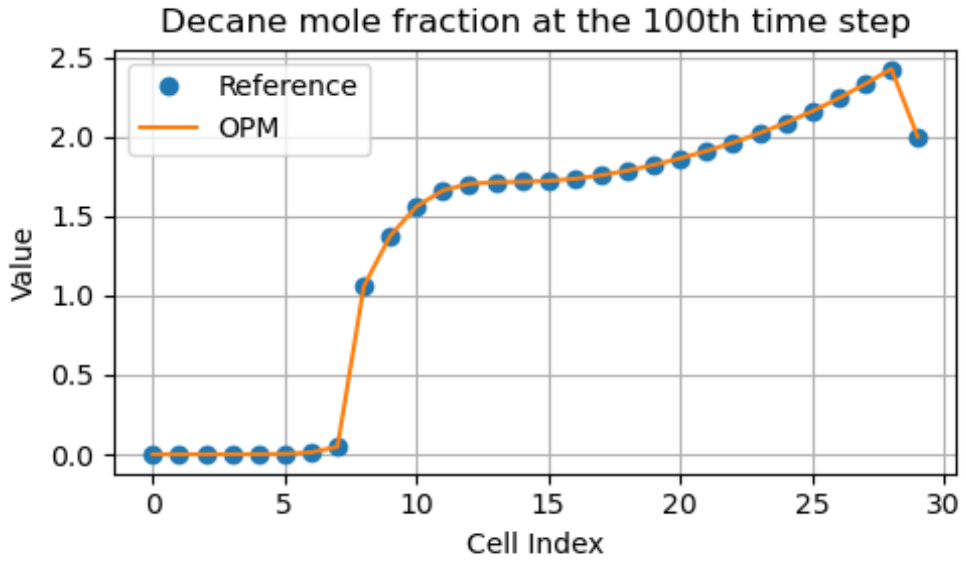


Validation against reference result







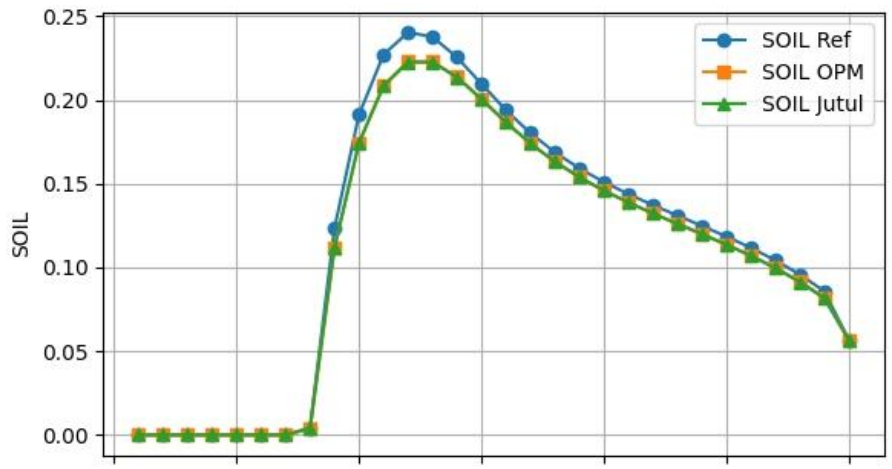


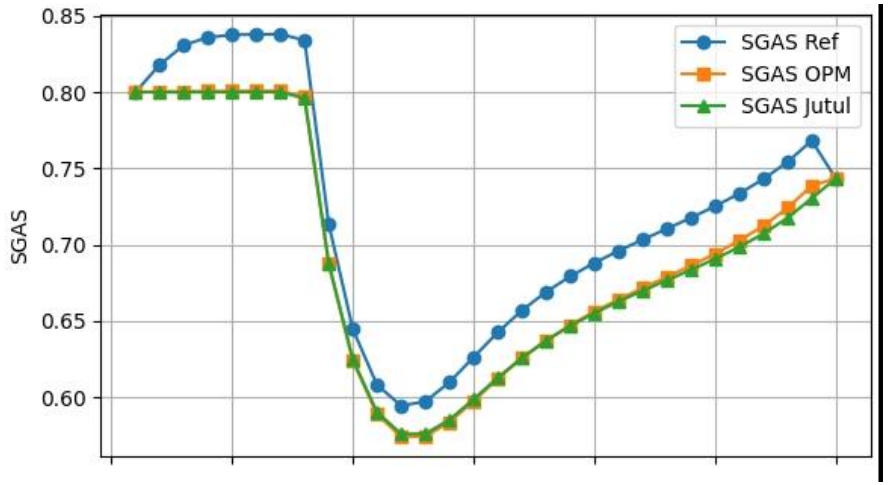
Test case 2

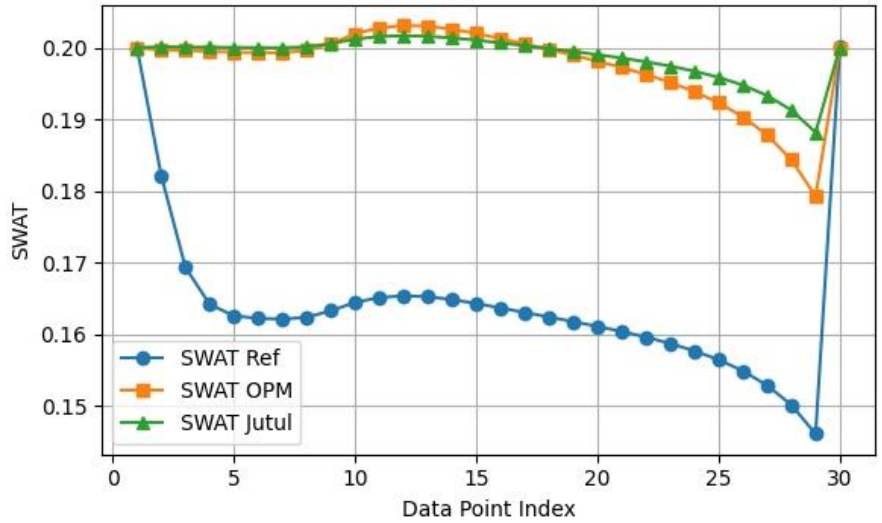
- Three phase with immiscible water phase
  - Same case with Test case 1, while we initialize with 0.2 water saturation

```
PRESSURE
1*150 28*75. 1*37.5
/
SGAS
30*0.8
/
SWAT
30*0.2
/
TEMPI
30*150
/
ZMF
1*0.99 29*0.5
1*0.009 29*0.3
1*0.001 29*0.2
/
```

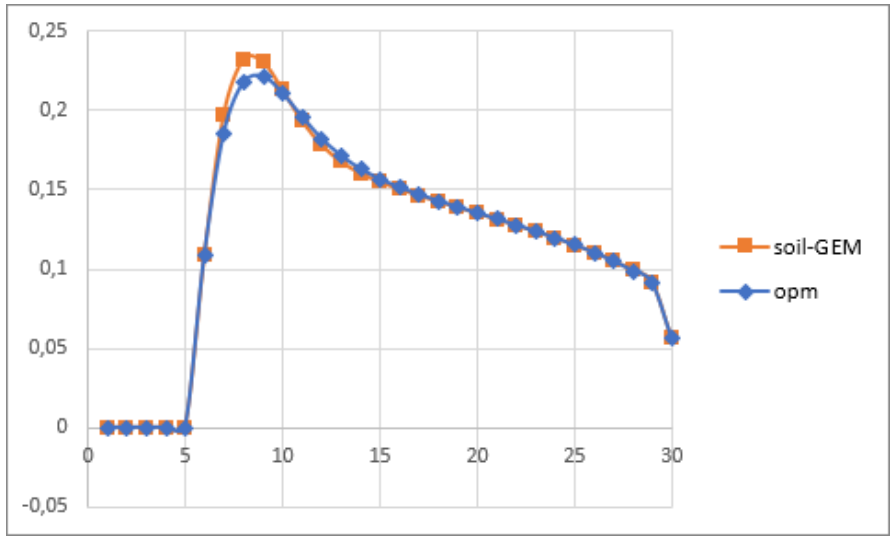
Comparison with reference simulators

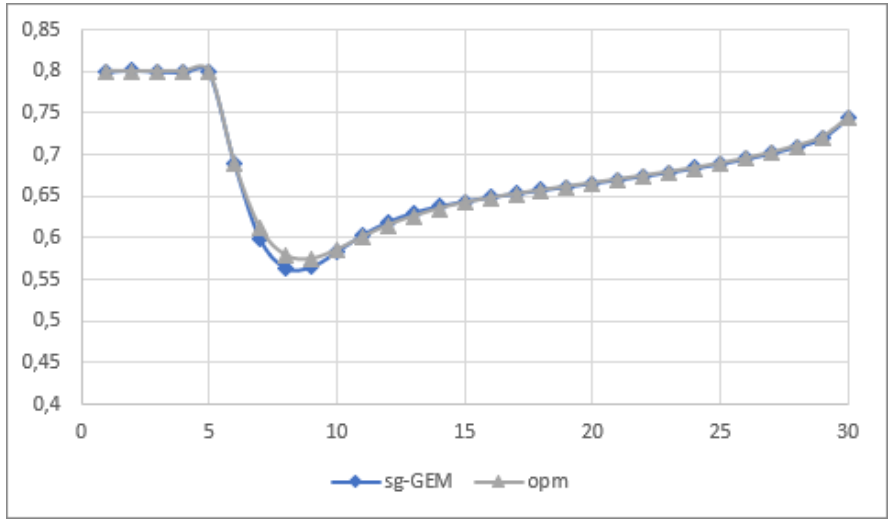


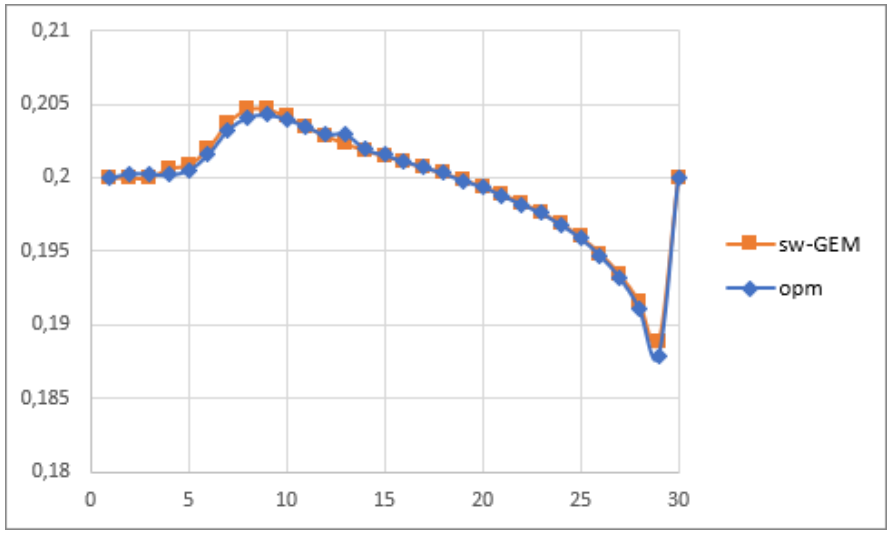




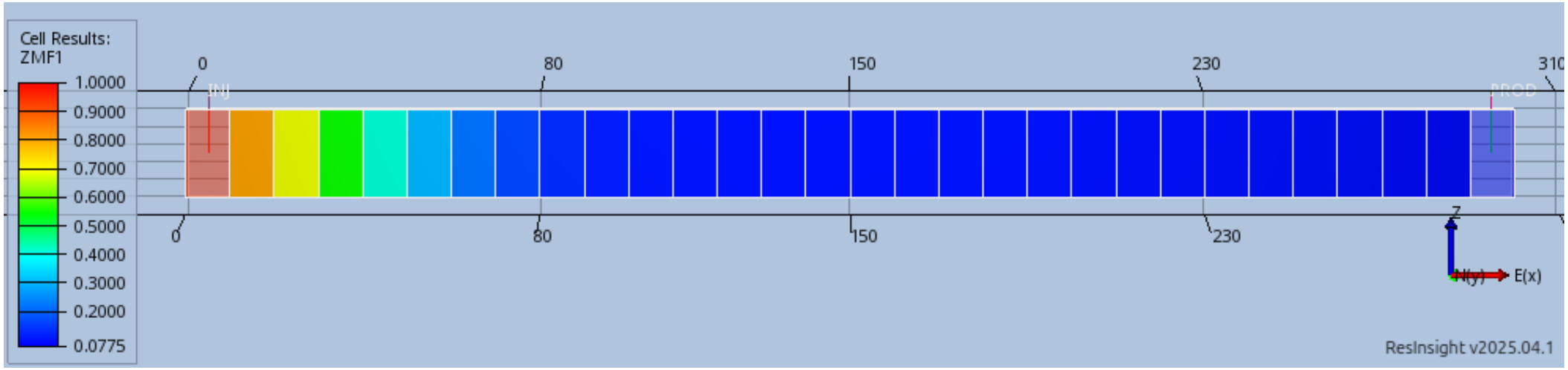
Comparison of the OPM and GEM



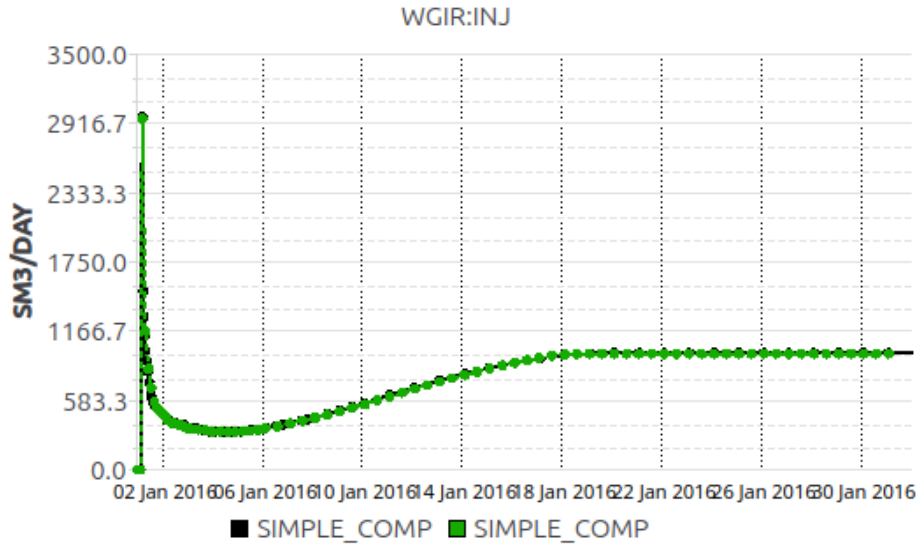


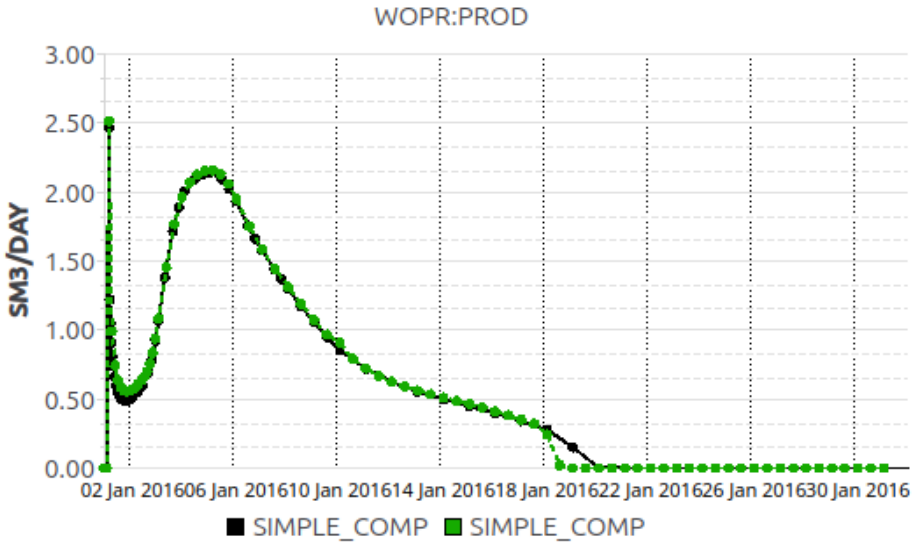


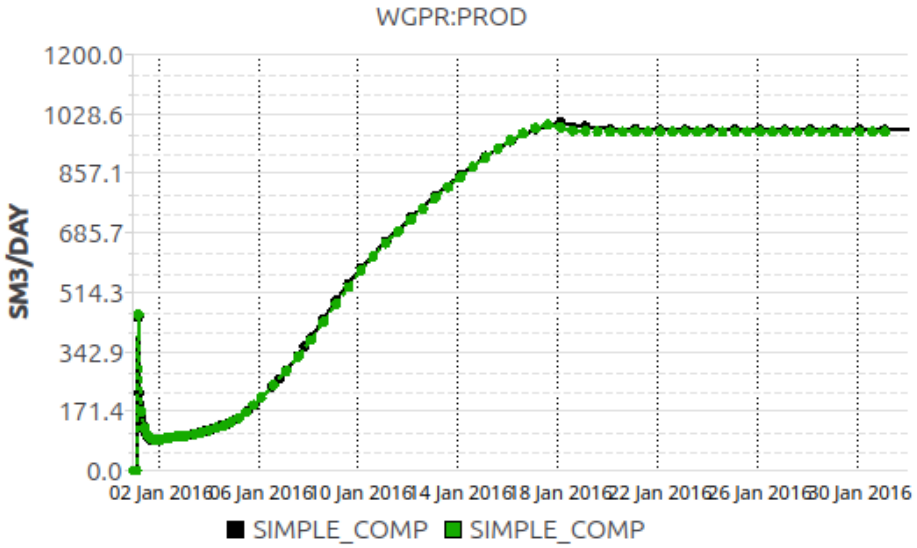
Test case 3 (simple well model)

- An injector and a producer
- The injector is injecting CO2 at BHP 150 bar with rate limit of 1.0e5 m^3/day.
- The producer is producing at BHP 50 bar with gas production rate limit of 1.0e5m^3/day.
- 

Summary plot with qsummary







Things can be next

- Evaluating the development/simulator to be more mature
  - More testing and robustness improvement
  - Features to make the simulator more applicable
    - Dynamic temperature, parallel solution strategy, equilibration for initialization, more general well modeling including multi-segment wells, and so on
  - Working with reservoir engineers to understand the needs more

- Other possible development
  - Enthalpy formulation for thermal injection, it can potentially elevate the OPM-flow more among different simulators

Summary

- The compositional simulator is still in the early stage, while a preliminary framework from DATA input to output is established
  - Equation of states, flash calculation, flow equations, well modelling, parsing and output
- It is readily elevated by incorporating existing capacities from flow simulator
  - Parsing, schedule, grid, parallelization, linear/nonlinear solvers, input/output facility, surface facility, time stepping, etc.
- As a more generic concept, it will help us to rethink the design of the black oil simulator and bring potential inspiration
- The development can be extended to handle both CCUS and hydrocarbon field.

Acknowledgement

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Thank you!