

# Compositional Simulation with OPM-flow

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# Contributors



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# A small history



- PT-Flash calculation June 2022
- 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
- Summary and Restart output Oct. 2024
- Compositional well modeling -> ongoing

# Compositional reservoir simulation

- Mass balance equations for N components

$$\frac{\mathbf{M}_i^{n+1} - \mathbf{M}_i^n}{\Delta t^n} + \text{div}(\mathbf{V}_i) - \mathbf{Q}_i = 0, \quad i \in \{1, \dots, N\}.$$

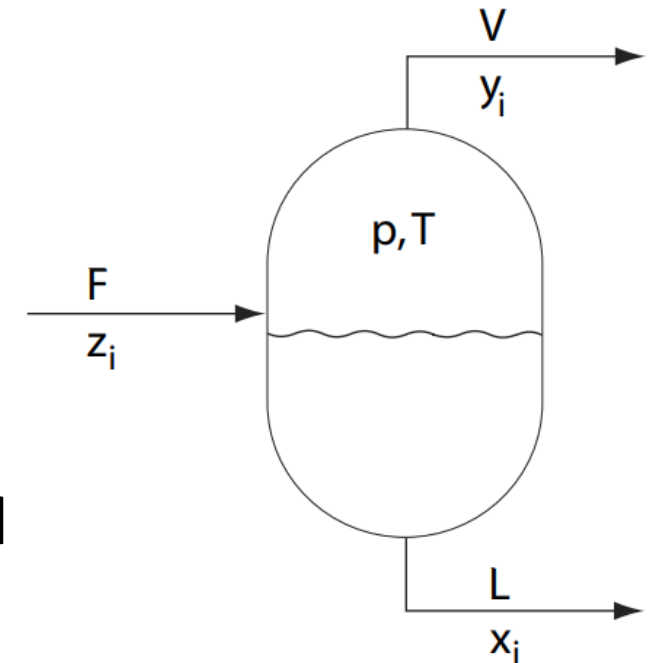
$$\mathbf{M}_i = \Phi (\rho_\ell S_\ell X_i + \rho_v S_v Y_i)$$

$$\mathbf{V}_i = -\mathbf{T}^f (\lambda_{i,\ell}^f \Theta_\ell + \lambda_{i,v}^f \Theta_v)$$

$$\sum_i^N x_i = 1, \quad \sum_i^N y_i = 1, \quad S_\ell + S_v = 1, \quad p_v = p_\ell + p_{cvl}$$

# Isothermal flash calculation

- Vapor Liquid two phase
  - fugacity equilibrium
- Peng-Robinson equation of states
- Stability test
- Successive substitution iteration (SSI), Newton method and Hybrid SSI-Newton
- Automatic differentiation (AD)



# Supported compositional keywords



- COMPS
- EOS
- CNAMEs
- ACF, MW, PCRT, TCRIT, VCRIT, BIC
  
- XMF, YMF, ZMF

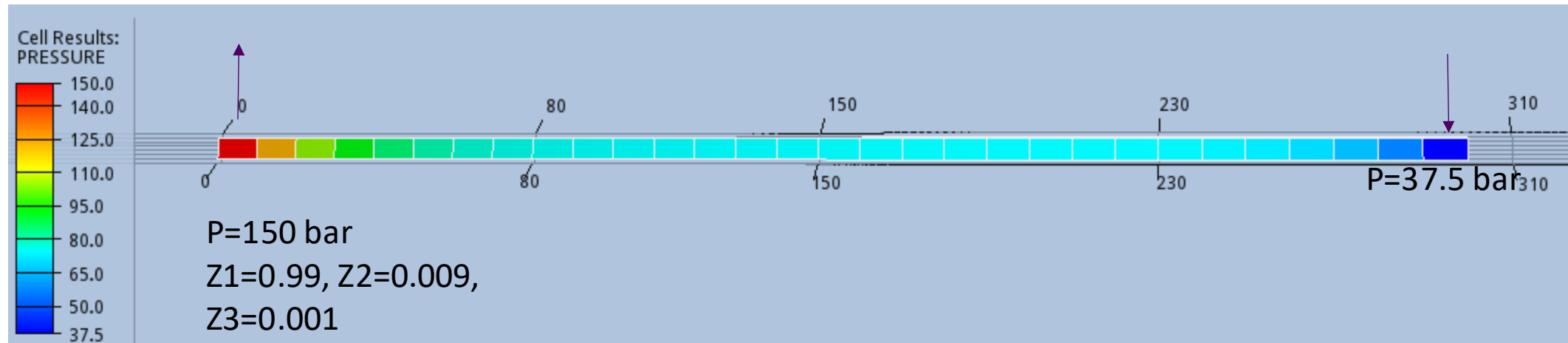
# Demonstration



- flowexp\_comp
- arguments:
  - --ecl-deck-file-name (input file)
  - --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 --ecl-deck-file-name=SIMPLE\_COMP\_SMALLZ.DATA  
--output-dir=outputdir --enable-vtk-output=true

# Test Case

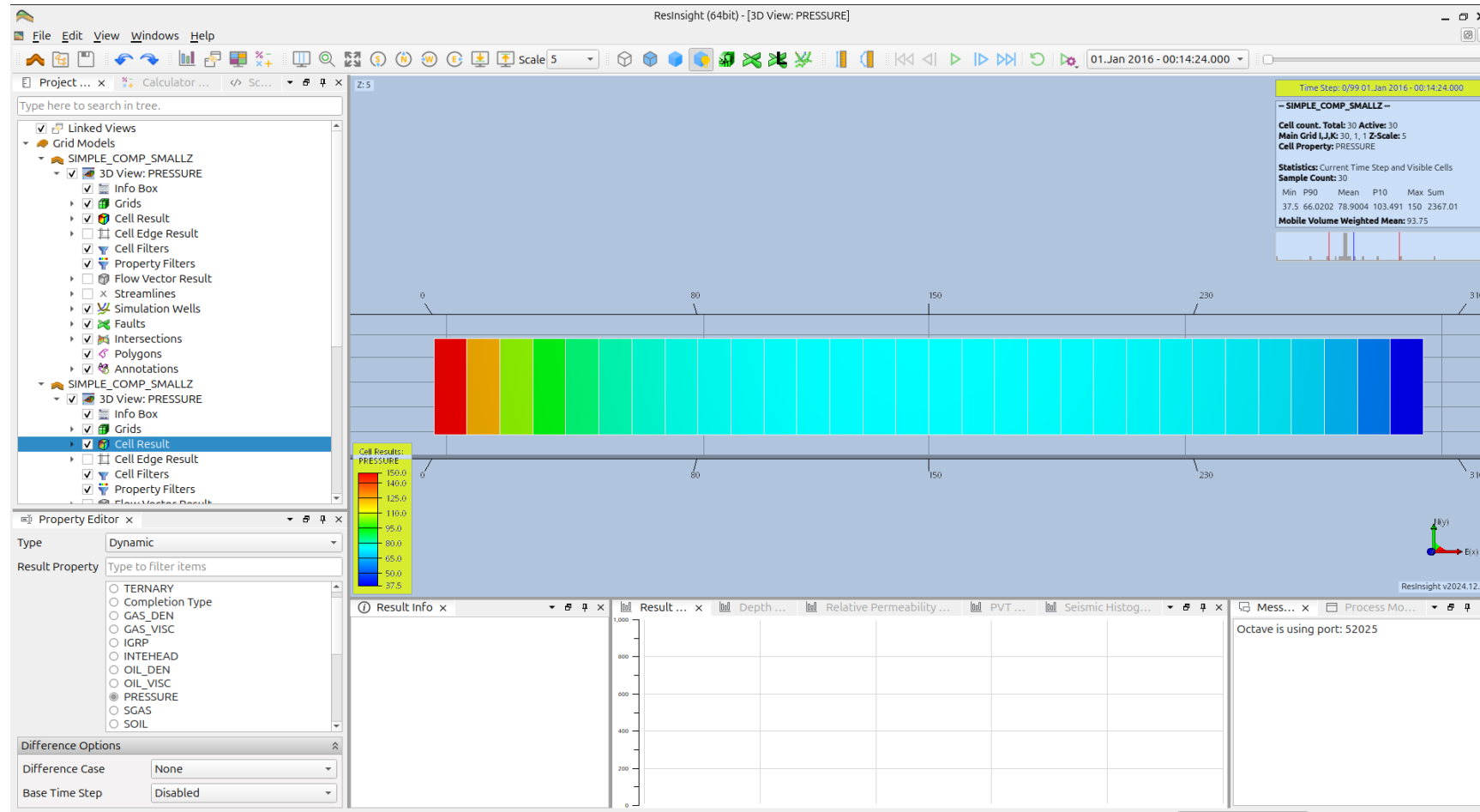
- 1-D model (30x1x1)
- $K=100$  mD,  $\Phi=0.1$ ,  $P_{res}=75$  bar,  $S_{Gas}=1$ ,  $T_{res}=150$  °C,
- Components (CO<sub>2</sub>(1), CH<sub>4</sub>(2), Decane(3)),  $Z_1=0.5$ ,  $Z_2=0.3$ ,  $Z_3=0.2$
- Cell(1,1,1) and cell(30,1,1) are assigned with much bigger pore volume to mimic source and sink with constant pressure and compositions





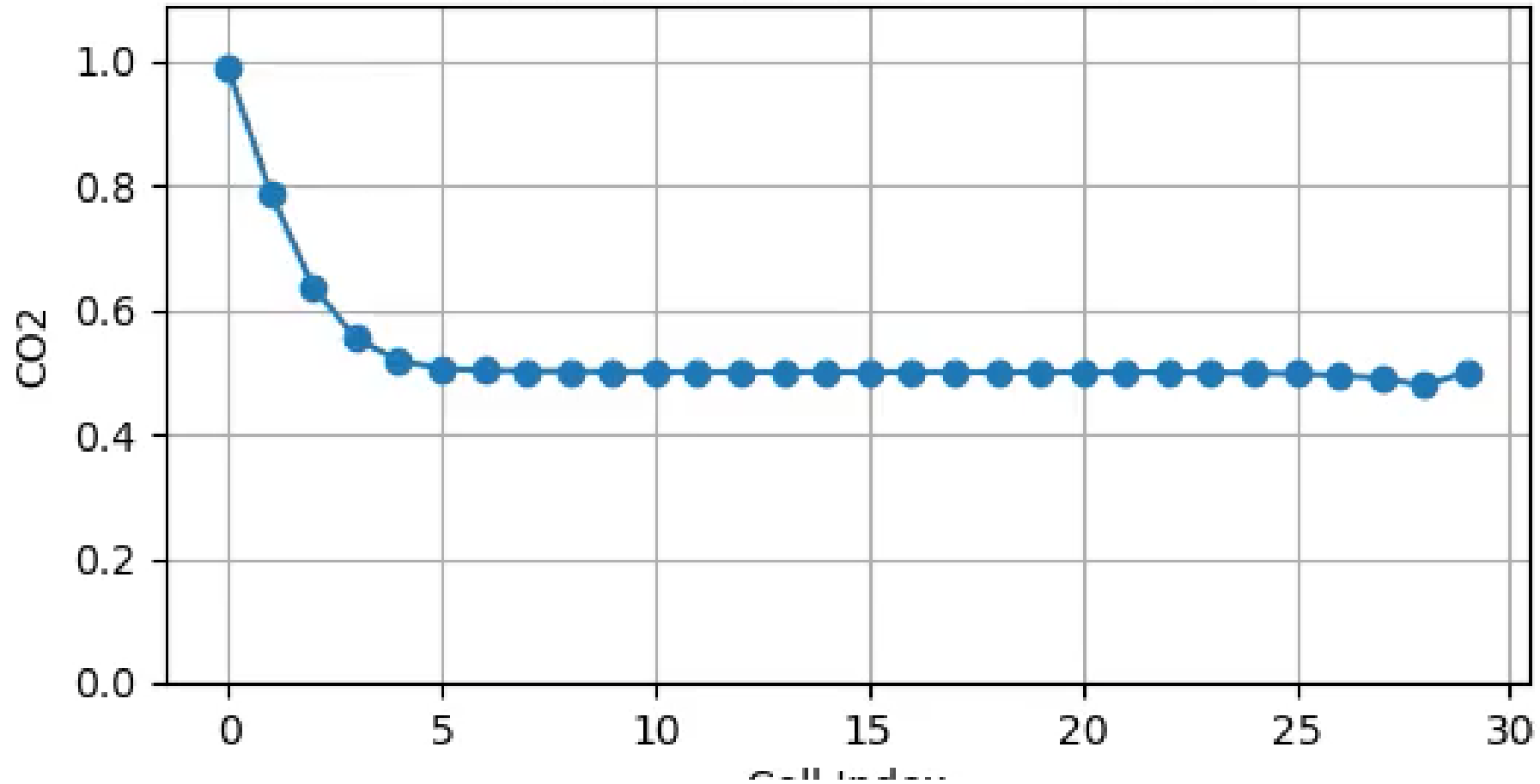
# Visualization

- ResInsight and Paraview can be used to visualize the output

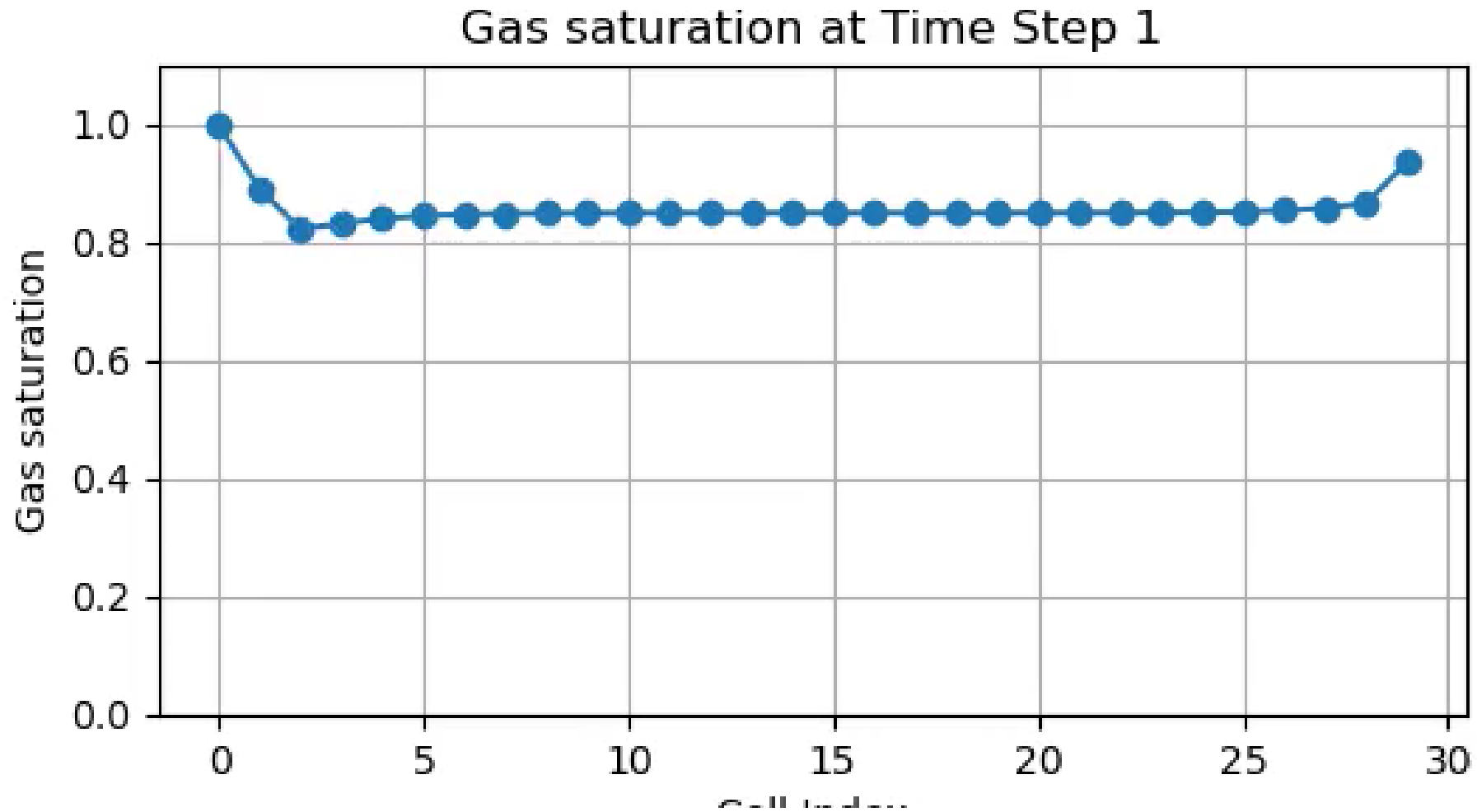


# Resulting CO2 mole fraction evolution

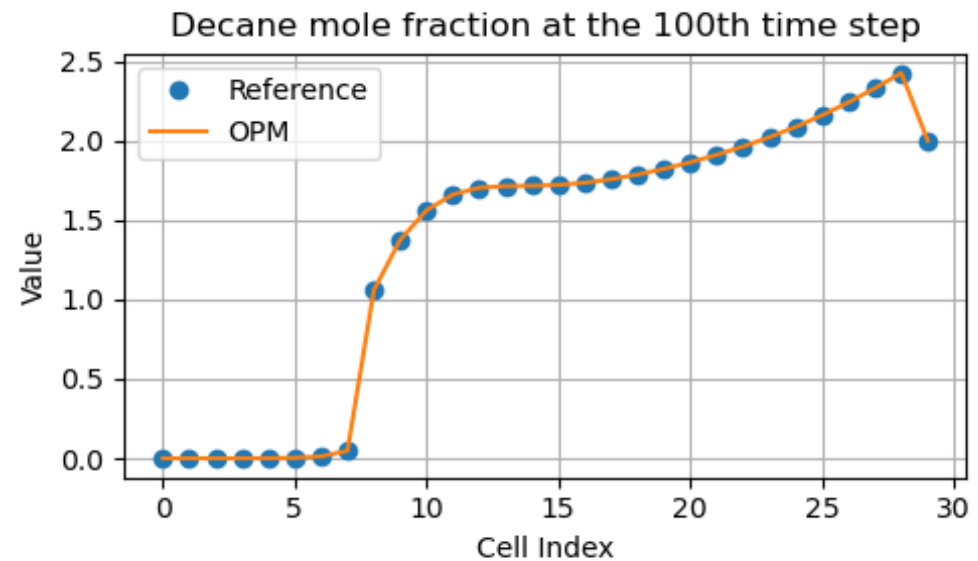
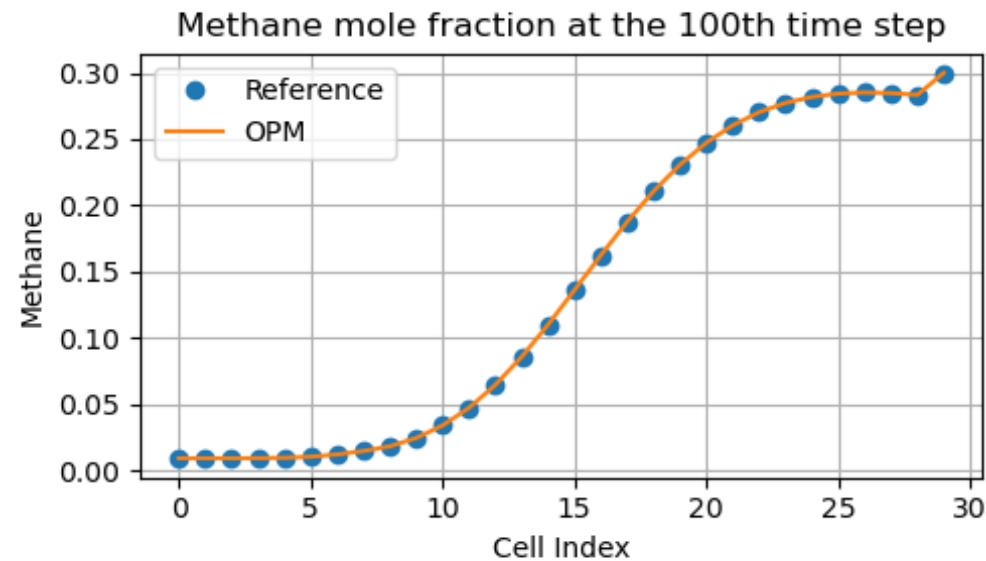
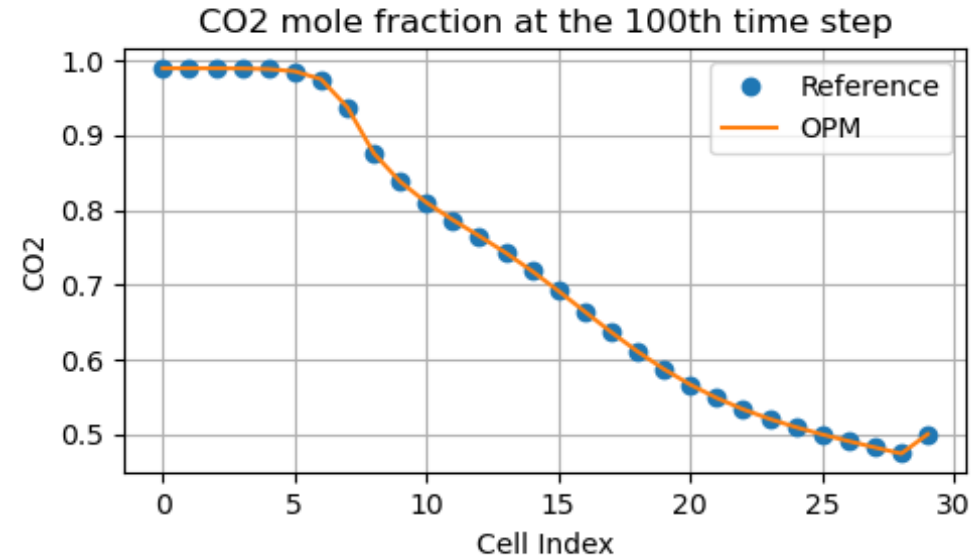
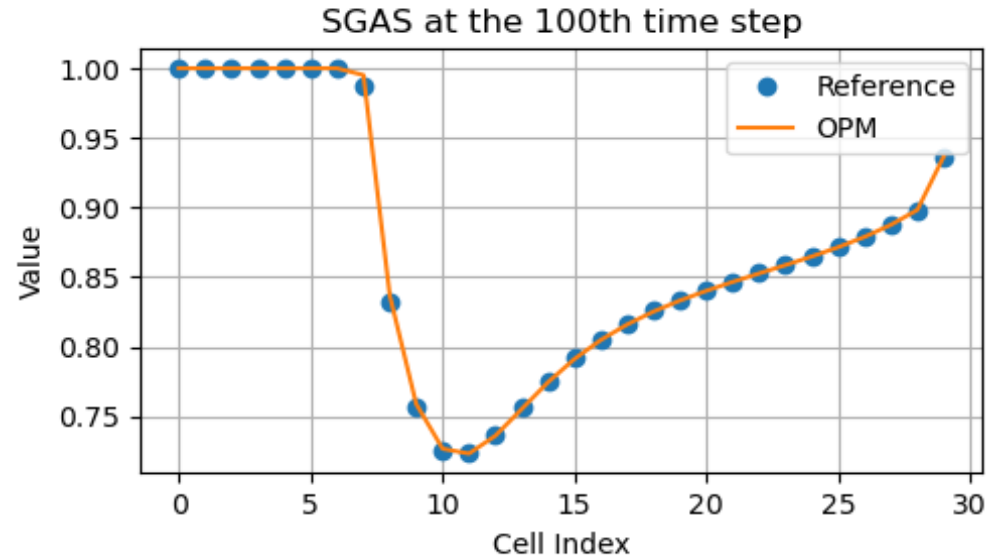
CO2 mole fraction at Time Step 1



# Resulting gas saturation evolution



# Validation against reference result



# Features expected for OPM Release 25.04



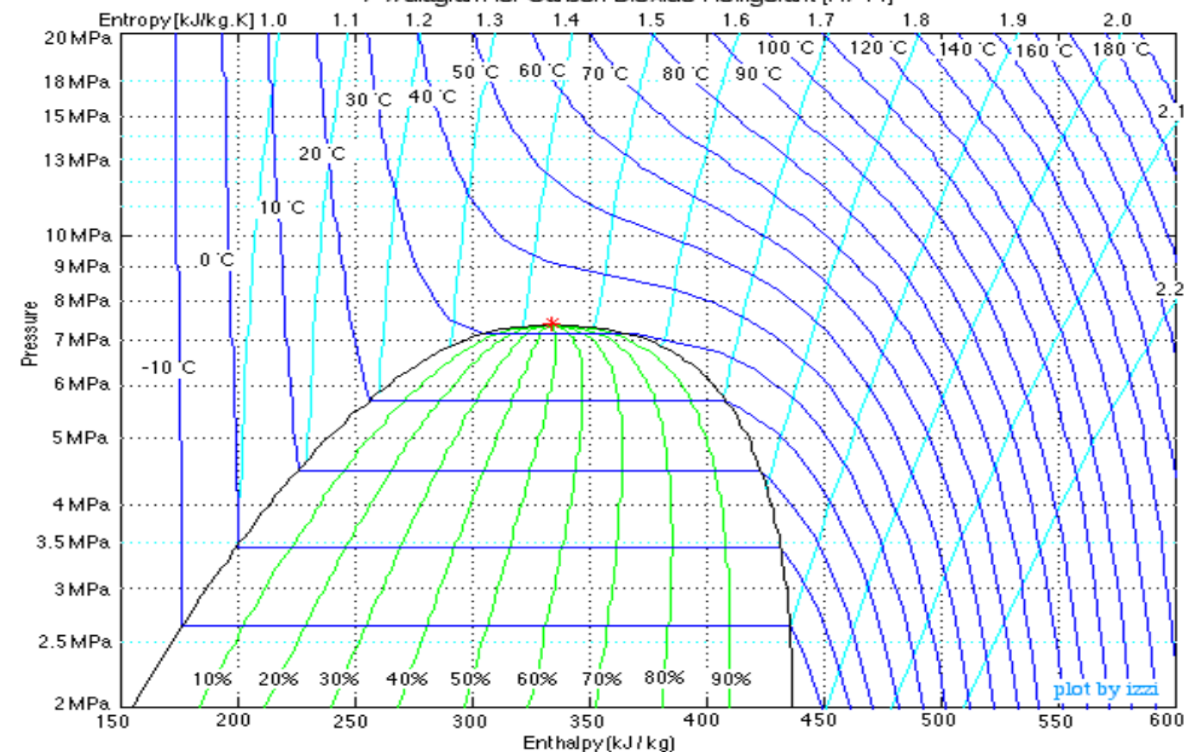
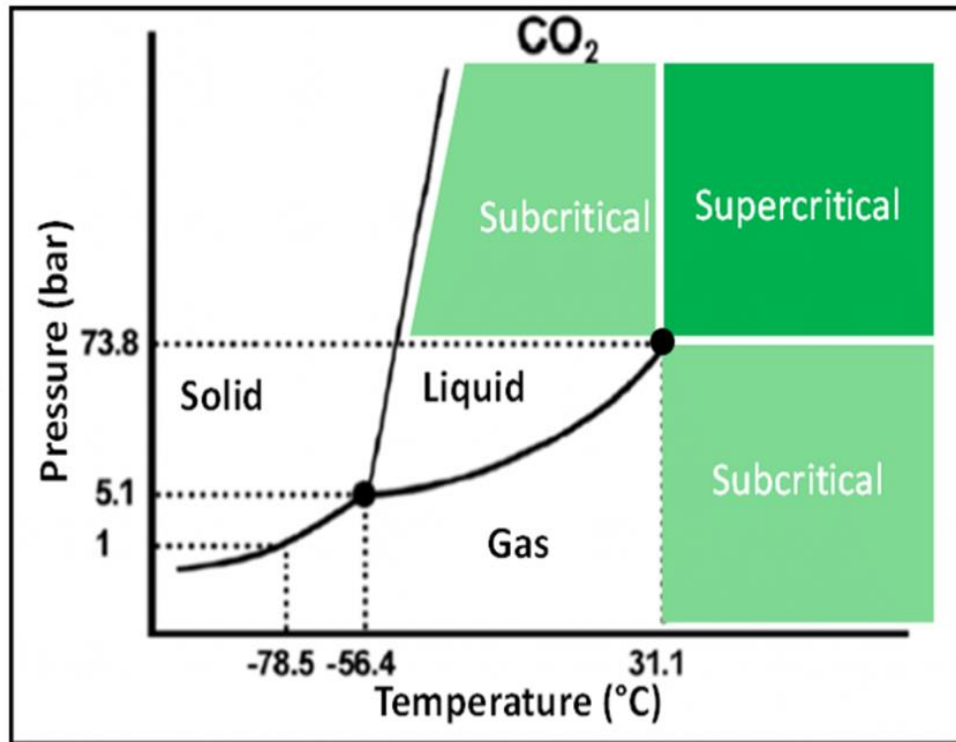
- Compositional Standard Well model (working in process)
- Three phase with water
  - water is not involved in flash calculation
- Equilibration initialization

Hopefully

- Testing with bigger models for CO2 injection
- Thermal

# EOS Based Thermal Compositional Energy Balance Formulation - Enthalpy Formulation

$$\frac{\partial}{\partial t} \left[ \phi \left( \sum_{j=1}^{np} \rho_j S_j U_j \right) + (1-\phi) \rho_r U_r \right] = -\nabla \cdot \left( \sum_{j=1}^{np} \rho_j h_j u_j \right) + \nabla \cdot (K_T \nabla T) + q_H$$



# Summary



- It is still in the early stage.
  - Testing, refactoring, optimization, adding features
- It can be readily elevated by incorporating existing capacities from flow simulator
  - Parsing, schedule, grid, parallelization, linear solvers, input/output facility, etc.
- It is on the way to be ready for future research and application.

Thank you!