



Contribution ID: 1001

Type: Poster Presentation

# A fully implicit single-phase multi-component phase transition pore network model based on automatic differentiation and GPU acceleration

*Monday, 13 May 2024 14:55 (1h 30m)*

The complex phase behavior of hydrocarbon mixtures is encountered in miscible flooding in the oil-saturated reservoir and liquid dropout in gas-condensate reservoir. In pore-network models, phase equilibrium calculations (Michelsen, 1982) have been coupled with convective-diffusion equations to evaluate the influence of hydrocarbon phase behaviors to flow and transport at given hydrocarbon mole compositions and temperature, as reported by Chen et al. (2020) and Santos, M.P.P.C. et al. (2020) where a fully implicit Euler method is implemented to get the set of non-linear algebraic equations at each time step solved by Newton's method. The number of convective-diffusion equations varies with pseudo-components number, which brings great inconvenience to the analytical programming of Jacobian matrix. In this work, the reverse derivation technique based on the chain derivation rule (Baydin et al., 2017) is applied to evaluate Jacobian matrix using an open source C++ library named fadbad++ and the program is comparable in time to the analytical programming of Jacobian matrix.

In addition, the GPU parallelization is promising to the numerical studies of multi-component flow and transport with computationally intensive nature. In our test, a graphic card RTX 3060 with 12GB memory together with CUDA library is used to speed up the steady-state and transient simulation process. The program is compared with the one running on a CPU i5-12400F with the Eigen mathematical library. The comparison results show that the acceleration rate can be about 5 times in the single-phase dynamic simulation with a pore network of 8000 pore elements, and about 10 times in the single-phase steady-state simulation with 2 million pore elements.

The coupled model is used for gas-condensate reservoir simulation to investigate the effect of droplets on gas production processes. In future work, a more efficient coupling way will be explored (Collins et al., 1992), and the existing model will be advanced to two-phase flow simulation (An et al., 2023).

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## References

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**Session Classification:** Poster

**Track Classification:** (MS07) Mathematical and numerical methods for multi-scale multi-physics, nonlinear coupled processes