The 35th Workshop on Mathematical Analysis for Nonlinear Phenomena

Room 223, Building C4 (Natural Science Building No. 5)
Kanazawa University, Kakuma Campus Kanazawa, 920-1192, Ishikawa, Japan

Monday, September 14, 2026 13:00–13:30

Alternative Formulations of Phase Stability Testing and Flash Equilibrium Calculation and their Applications in Compositional Simulation

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In this talk, I am going to present various formulations of two basic problems in the thermodynamics of multicomponent mixtures, namely the global phase stability problem and the phase equilibrium calculation problem (also called flash equilibrium calculation). The traditional formulations are based on the specification of the pressure P, temperature T, and overall mole numbers N_i. In the phase stability problem, we seek whether a mixture of n components at pressure P, temperature T, and mole numbers N_i $(i = 1, \ldots, n)$ stays homogeneous (single-phase) or splits into two (or more) phases. If the system splits, then the phase equilibrium calculation is performed to determine the number of phases, their compositions, densities, and phase amounts. However, both problems can be formulated under other variable specifications as well. I will present the alternative variable specifications VTN (volume, temperature, and moles) and UVN (internal energy, volume, and moles). I will show that all these three formulations can be reformulated under one unifying framework and a single code can be written that can treat all these specifications. Various examples of calculations of multicomponent mixtures will be presented. In the final part of the talk, I will discuss advantageous features of the alternative formulations based on the other variable specifications and show their usefulness in compositional simulations. I will also mention some ongoing work and directions for further research and possible collaborations.

This is a joint work with Tomáš Smejkal (CTU), Ondřej Polívka (CTU), Tereza Petříková (CTU), Abbas Firoozabadi (Reservoir Engineering Research Institute, Palo Alto, CA, USA), Martin Jex (CTU), and Petr Gális (CTU).

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A Thermo-Poro-Elastic Phase-Field Model for Hydraulic Fracturing

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Fluid-driven fracture propagation in porous media is a key process in hydraulic stimulation, geothermal energy extraction, and subsurface engineering, requiring models that capture the interplay between mechanical deformation, fluid transport, and thermal effects. This work presents a coupled thermo-poro-mechanical phase-field 2D model for hydraulic fracturing in brittle porous media. The model couples linear-elastic solid mechanics (with a tension–compression energy split), Biot poroelastic fluid flow, a thermal energy balance, and a phase-field description of fracture based on the Ambrosio–Tortorelli/Bourdin regularization, with irreversibility enforced via a strain-history field. Effective material properties transition smoothly between rock and fracture through phase-field-based indicators. The system is discretized using the standard continuous Galerkin finite element method for elasticity and the temperature evolution equation, together with a mixed finite element method for the pressure equation (mass balance) and phase-field equation. SUPG stabilization is applied to the temperature equation due to the advection-dominated regime of the fluid flow.

This work is based on [1].

This is a joint work with Professor Jiří Mikyška (CTU, Czech Republic) and Professor Abbas Firoozabadi (Rice University, USA).

[1] Y. Feng and A. Firoozabadi, *Phase-Field Simulation of Hydraulic Fracturing by CO_2 and Water with Consideration of Thermoporoelasticity*, *Rock Mechanics and Rock Engineering*, 56 (2023), 7333–7365. DOI: 10.1007/s00603-023-03365-7.