Operator-Based Linearization approach for flow and transport with equilibrium and kinetic reactions

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Increasing demand for energy sources, e.g. complex hydrocarbon reservoirs or geothermal energy, has led to the comprehensive investigation of carbonate reservoirs. These reservoirs are often chemically altered and hence contain a large uncertainty in the spatial distribution of the reservoir parameters. A successful development of these cleaner energy resources and effective management of the associated risks requires an evaluation of the large ensemble of multiphase reactive flow and transport simulations. To solve this problem, we developed an efficient element based reduction technique which can significantly decrease the number of conservation equations and thereby reduce the computational time.

The proposed formulation is based on the consistent element balance reduction of the molar (overall composition) formulation [1]. To predict the complex phase behavior in such systems, we include the chemical equilibrium constraints to the multiphase multi-component negative flash calculations and solve the thermodynamic and chemical phase equilibrium simultaneously [2]. In this solution, the phase equilibrium is represented by the partition coefficients whereas the chemical equilibrium reaction is represented by the activity coefficients model. This provides a generic treatment of chemical and thermodynamic equilibrium within the successive substitution loop of multiphase flash to accommodate precipitation and dissolution. Using the Equilibrium Rate Annihilation matrix allows us to reduce the governing unknowns to the element conservation equations only while the coupling between chemical and thermodynamic equilibrium is captured by a simultaneous solution of modified multiphase flash equations. The element composition of the mixture serves as an input for these computations whereas the output is fractions of components in each phase, including solids.

Next, a finite-volume unstructured discretization in space is applied together with a fully-implicit approximation in time. The resulting complex nonlinear system is parameterized using the Operator-Based Linearization (OBL) approach [3]. The OBL framework transfer the governing nonlinear Partial Differential Equations into a linearized operator-form where the Jacobian is constructed as a product of a matrix of derivatives with respect to state variables and discretization operators. The state-dependent operators are only evaluated adaptively at vertices of the mesh introduced in the parameter-space. The continuous representation of state-dependent operators as well as their derivatives is achieved by using a multi-linear interpolation in parameter-space. This means that the usually time-consuming phase and chemical equilibrium computations, performed on each nonlinear iteration and in every control volume, are only executed when evaluating the operators in the new supporting points, thereby significantly reducing both the linearization time and the number of nonlinear iterations. The simulation of multidimensional problems of practical interest has been performed using the proposed technique. The same approach is later used to simulate the near-wellbore mineral precipitation prevalent in North Sea gas reservoirs.

Equilibrium reactions in typical advection-diffusion problems are usually valid when the rate of the reaction is far greater than characteristic velocity or diffusion. This is typically not true when considering heterogeneous reactions such as complex dissolution/precipitation processes. Therefore, a kinetic reaction module has also been developed within the OBL approach. The newly added module in the OBL framework for multiphase reactive transport and flow is validated for several dissolution regimes at different combination of Damkohler and Peclet numbers. The element based reduction framework, using equilibrium reactions, is compared with the component kinetic reaction framework at different kinetic rates.

References

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