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Editorial

A 6M digital twin for modeling and simulation in subsurface reservoirs

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Modeling and simulation of flow, transport and geomechanics in the subsurface porous media is an effective approach to help make decisions associated with the management of subsurface oil and gas reservoirs, as well as in other wide application areas including groundwater contamination and carbon sequestration. Accurate modeling and efficient, robust simulation have always been the main purposes of reservoir researches, and a 6M digital twin (multi-scale, multi-domain, multi-physics and multi-numerics numerical modeling and simulation of multi-component and multi-phase fluid flow in porous media) is designed, equipped with the following six pronounced features, to better digitally model and simulate the engineering processes and procedures in physical reality and further control and optimize such processes and procedures:

1. Efficient and reliable flash calculation: An accurate estimation on the phase equilibrium conditions is essentially needed prior to multi-phase flow and transport simulation for multi-component fluid mixtures in complex porous geometry and thermodynamic conditions. A remarkable progress was recognized in 2018, when a thermodynamically stable multi-phase equilibrium calculation algorithm of hydrocarbon mixtures based on realistic equation of state (e.g., Peng-Robinson Equation of State) at specified moles, volume and temperature (NVT-flash) was generated and proposed (Kou and Sun, 2018a, 2018b; Sun, 2019). Robustness of this algorithm is preserved by proved consistency with the first and second laws of thermodynamics and capillarity can be incorporated in this algorithm to extend the application into unconventional reservoirs (e.g., shale gas reservoirs and tight oil reservoirs) and carbon dioxide sequestration (with cubic-plus-association type of equation of states) (Zhang et al., 2019a, 2019b; Li et al., 2020). Sparse grids method and parallel computing techniques have been involved in further studies to accelerate the phase equilibrium estimation on parallel computers (Wu et al., 2015a). Recently, deep learning algorithms have been successfully developed to significantly speed up the multi-component flash calculations in complex thermodynamic conditions at the same time of ensuring stability and self-adaptivity (Li et al., 2019a, 2019b; Zhang et al., 2019c, 2020a).

2. Advanced phase interface modeling: In multiphase flow simulation in porous media, modeling of the thin interface, usually in nanoscale thickness, is recognized as the key issue in order to simulate macroscale fluid behaviors containing the formation and motion of interphase. The multi-component multi-phase flow can be investigated using a diffuse interface model based on realistic equations of state (typically Peng-Robinson equation of state), and bulk phase properties as well as interfacial properties could be modeled accurately and efficiently, where partial immiscibility can be considered to cover more engineering applications like carbon dioxide in oil (Qiao and Sun, 2014; Kou et al., 2018). Based on that, a new momentum balance equation was proposed in Kou and Sun (2018c) to identify the correlation associating the gradients of temperature and chemical potential and the pressure gradient, which further indicates that the gradient of the temperature and chemical potential has been found as the primary driving force of the macroscale fluid motions. Later, phase field modeling was incorporated with the moving contact line method to study the motion of soluble surfactants using two Chan-Hilliard type

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of equations, which are designed to govern the surfactant concentration and interface evolution respectively (Zhu et al., 2019). Recently, a semi-implicit scheme was proposed in Kou et al. (2020) to generate for the first time a scheme that inherits the original energy dissipation law, using a delicate novel energy factorization (EF) approach to factorize an energy function into a product of several factors. Application of phase field modeling has been extended to a wider range in the whole process of petroleum engineering. An exploratory phase-field model was presented in Zhang et al. (2020b) to simulate the multiphase flow in injection pipeline investigating the effect of injection salinity on pipeline scaling.

3. Fully conservative bound-preserving Darcys scale flow simulation: Fully mass-conservative (both globally and locally, for wetting phase and non-wetting phase) IMPES (IMplicit Pressure Explicit Saturation) schemes for the simulation of incompressible and immiscible two-phase flow in porous media were generated in (Chen et al., 2019), which deserves a merit that a new treatment of capillarity was introduced and the unbiased and the bound-preserving property can provide a much larger time step choice. Furthermore, a nonlinear complementarity problem was reformulated and the resultant non-smooth nonlinear system of equations arising at each time step are solved fully implicitly by a parallel, scalable, and nonlinearly preconditioned semi-smooth Newton algorithm (Yang et al., 2019a). Later, a new scheme containing up to three continuity equations were generated in Yang et al. (2020) so that mass conservation holds for all present phases. By using a variational inequality formulation with box inequality constraints, boundedness requirement on pressure and saturations can be preserved well and then the problem is solved using a well-designed nonlinear solver consisting of the nonlinear elimination preconditioning technique and active-set reduced-space method.

4. Reactive flow and transport in porous media: Reactive dissolution of carbonates by the action of the injected acid, also known as wormhole propagation, is a widely practiced technique in the product enhancement of petroleum industry. A semi-analytic scheme was proposed with a reconstruction of analytical porosity functions to analyze the time error of the porosity, and a coupled analysis approach was employed to achieve the estimates of pressure, velocity and solute concentration on the basis of porosity error estimation (Wu et al., 2015b; Kou et al., 2019). Meanwhile, various primal discontinuous Galerkin schemes, including NIPG, SIPG and IIPG have been investigated deeply for solving multi-component reactive transport and coupled with multiphase flow simulation in porous media (Sun and Wheeler, 2005, 2006).

5. Molecular simulation of microscopic mechanisms: As an effective approach to investigate the microscopic mechanisms affecting macroscopic flow and transport behaviors as well as to obtain the value of key parameters in numerical modeling, molecular simulation has attracted increasing attentions. The diffusion and sorption behaviors of carbon dioxide and methane as well as the structural features were studied using molecular dynamics and hybrid Monte Carlo approaches (Kadoura et al., 2017; Yang et al., 2017a, 2019b). The intercalation behavior of carbon dioxide in various brines were studied using grand canonical Monte Carlo methods to study the molecular mechanisms indicating that the intercalation of carbon dioxide strongly depends on the relative humidity (Li et al., 2019c).

6. High-performance computation based on fully-Implicit and bound-preserving algorithms: Bound-preserving discretization and solvers for subsurface flow models based on a fully implicit framework is the future of parallel reservoir simulation (Yang et al., 2019a, 2020). A family of mixed finite element methods have been used to discretize various model equations in porous media flow for the spatial terms, and the implicit backward Euler scheme with adaptive time stepping for the temporal integration. The resultant nonlinear system arising at each time step was then solved in a monolithic way by using a Newton–Krylov type method, where the resultant nonlinear system was solved by a generalized Newton method, i.e., active-set reduced-space method, and then the ill-conditioned linear Jacobian systems were solved with an effective preconditioned Krylov subspace method. The used nonlinear preconditioner was built by applying overlapping additive Schwarz type domain decomposition and nonlinear elimination. Numerical results on parallel computers indicated that the nonlinear solver overcomes the severe limits on the time step associated with conventional methods, and it results in superior convergence performance, often reducing the total computing time by more than one order of magnitude (Yang et al., 2016, 2017b, 2018).

Conflict of interest

The authors declare no competing interest.

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