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Comprehensive comparison between kinetic and equilibrium models in simulation of hydrate reaction in porous media

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Coupling hydrate reaction in fluid transport in porous media is essential for simulation of gas hydrate production, as well as carbon sequestration in deep-sea sediments. Hydrate reaction in porous media can be conceptualized as multiphase, multicomponent and non-isothermal reactive transport. Two types of models have been developed for hydrate reaction in numerical model. Equilibrium model (EM) assumes instantaneous chemical equilibrium among species and thus ignores the reaction kinetics. Kinetic model (KM) incorporates the reaction kinetics by introducing a term of reaction rate dependent on fugacity difference. Although KM has a more accurate description of reaction, it is more computationally intensive due to the increased degree of freedom in the nonlinear equation system. Several previous studies have investigated the similarities and differences between these two models through case studies and sensitivity analysis, however, most of the results and conclusions remain qualitative. In our study, via theoretical analysis and numerical studies, we provide comprehensive comparison between these two reaction models. Through comparing the basic assumptions and equation systems, we analyze thoroughly the differences between these two models. Dimensionless analysis of the equation system of KM yields several characteristic numbers, representing the relative strength of different physical processes. It is found that there exist critical values for theses characteristic numbers, exceeding which leads to an obvious gap between the results of EM and KM. It turns out that the relative strength of the physical processes controls the magnitude of difference between these two models. EM is essentially a special case of KM when the time scale of hydrate reaction is sufficiently smaller than other physical processes such as convective and diffusive transport of mass and heat. Based on this conclusion, we investigate the impact of different parameters on the difference between EM and KM, such as permeability, porosity, phase saturations, formation pressure and temperature, and reaction related parameters. Finally, we provide suitable ranges of characteristic numbers for using equilibrium model.