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Thermodynamics-Informed Neural Network for Phase Equilibrium in Subsurface Reservoirs

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Multi-phase multi-component flows are the key problems needing to be solved in the study of subsurface geological formation and fluid flows, which are essentially required in the understanding and description of complicated heat and mass transfer behaviors commonly seen in oil and gas reservoirs. A large number of chemical species have been detected in the reservoir fluids, which challenges the conventional computational multi-phase fluid dynamic simulation using empirical formulas. The number of phases existing in the fluid mixture, as well as the phase partitioning information of each component, play an important role in the multi-component multi-phase model and simulation to keep the thermodynamic consistency and physical meaningfulness. Flash calculation, the main approach to obtain these information, including overall density, chemical composition and the total phase numbers at equilibrium, has shown its inevitability in energy discovery and recovery, especially when the concept of Enhanced Oil Recovery (EOR) is discussed. Recently we demonstrated that the deep neural network models, while preserving high accuracy, are more than two hundred times faster than the conventional flash algorithms for multicomponent mixtures. Previous machine learning methods assume a fixed number of components in the fluid mixture, which makes such models to have very limited practical usefulness. In this work, we propose to develop self-adaptive deep learning methods for general flash calculations, which can automatically determine the total number of phases existing in the multicomponent fluid mixture and related thermodynamic properties at equilibrium. Our preliminary work showed that, for example, the deep learning model with the 8-component Eagle Ford oil flash calculation results as training data accurately predicts the phase equilibrium properties of a 14-component Eagle Ford fluid mixture.

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