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Machine Learning Assisted Numerical simulation of Propylene Glycol-mixed Steam Enhanced Extraction in Unsaturated soils

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Contaminated soils with hazardous persistent organic pollutants, such as Polycyclic Aromatic Hydrocarbons (PAHs), present significant challenges for efficient remediation, attributable to their low mobility and bioavailability. The technique of Propylene Glycol (PG)-mixed steam enhanced extraction has emerged as a promising remediation technology, markedly increasing the solubilization and desorption of PAHs through the application of condensed PG and input enthalpy. Despite its potential, a comprehensive understanding of the heat and mass transfer dynamics during PG-mixed steam injection remains conspicuously underexplored, a gap critical to determining the technology's remediation scope and efficacy. In this study, a compositional two-phase flow model was constructed to elucidate the heat and mass transfer mechanisms in unsaturated soils subjected to PG-mixed steam injection, utilizing the Dumux framework. To account for the chemical equilibrium of water, PG, and air across both gas and liquid phases, the 'feos' toolbox was employed for phase equilibrium and thermodynamic property calculations, enabling the determination of the fugacity coefficients for the various components in the liquid phase. Simultaneously, the behavior of gas-phase components was modeled as an ideal gas. A multi-layer neural network was developed and trained to predict the fugacity coefficients of these components under diverse conditions, including variations in temperature, pressure, and liquid-phase composition. This model serves as a novel approach to provide fugacity coefficients, facilitating the computation of the mole fraction of each component in both phases. Comparative results indicate that the machine learning model substantially enhances computational efficiency relative to tabulated searches for fugacity coefficients. The model yields plausible predictions of temperature and pressure variations, as well as the distribution of water and PG across both phases, surpassing the traditional assumption of an ideal PG-water solution. Subsequent sensitivity analysis will delineate pivotal parameters governing heat and mass transfer during PG-mixed steam injection, identifying critical operational zones. Overall, this numerical model is instrumental in advancing the understanding of PG-mixed steam enhanced extraction processes and serves as a foundational reference for engineering design.

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