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Uphill diffusion and phase separation in partially miscible multicomponent mixtures[1] PING HE, ASHWIN RAGHAVAN, AHMED GHONIEM, Massachusetts Inst of Tech-MIT — The partially miscible multicomponent mixtures, which are frequently encountered in green chemistry processes, often exhibit complicated behaviors, and are critical to the production rate, energy efficiency, and pollution controls. Recent studies have been mainly focused on phase behaviors. However, the coupled phase equilibrium and transport process, which may be the answer to phase separations observed in experiments, is not well researched. Here, we present a numerical and theoretical study on coupled mixing of heavy oil and supercritical water, and the results of our state-of-art modeling agree with experimental measurements. We find that due to the non-ideal diffusion driving force, (1) strong uphill diffusion of heavy oil fractions occurs, (2) a new heavy oil phase is separated starting from the plait point, and heavy fractions become highly concentrated, and (3) water diffusion initially overshoots in oil, and is expelled lately. Finally, we conclude our analysis applicable to different molecules and conditions.

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