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The effect of temperature heterogeneities on the dynamics of reactive ternary systems CHRISTOPHER POOLEY, ANNA BALAZS, University of Pittsburgh — We investigate the the role of one of the most important processing variables, namely temperature, on the structural evolution and phase behavior of a complex fluid. Using a lattice Boltzmann algorithm we numerically study the behavior of a partially miscible A/B/C ternary mixture. Within the simulations we explicitly account for fluid flow, phase separation and heat transfer. In particular, we study a system in which the A and B components can reversibly react to produce C. Such reactions involve the liberation and consumption of heat, which alters the local thermodynamic equilibrium near to the interfaces between components. Since the reaction rates themselves are temperature dependent there exists a coupling between compositional and thermal variation within the system, which leads to interesting dynamical behavior. In addition, we investigate how the morphology depends upon laterally applied temperature gradients. With these simulations we take the first steps in capturing the complex compositional and thermal heterogeneities inherently present in chemical reaction vessels.

Christopher Pooley
University of Pittsburgh

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