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**LATTICE BOLTZMANN METHOD FOR MULTIPHASE REACTING FLOWS
WITH CHEMICAL INDUSTRY APPLICATIONS**

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PROJECT SUMMARY

The overall objective of this SBIR project is to develop an innovative and efficient computational package based on the lattice Boltzmann method (LBM) for multiphase reacting flows in chemical engineering applications. In Phase I, a three-dimensional (3D) LBM for multiphase flows with high phase-density ratios based on phase-field models is developed. The phase-field/LBM, based on the concepts of free-energy functionals, has better physical consistency in recovering multiphase flow behavior and is computationally more efficient than earlier LBM approaches. Assessments of the phase-field/LBM for a set of canonical multiphase flow problems show good agreement with prior work. Another important element developed in Phase I is a computational procedure for transport of passive scalars including chemical reactions based on the so-called total variation diminishing (TVD) scheme. Through employing flux limiter concepts and using the velocity field from the LBM, the TVD scheme significantly reduces numerical effects, such as spurious dispersion, from affecting the physical solution of the transport of passive scalars in the presence of sharp gradients and/or changes in physical properties. The computed results based on the TVD scheme for a series of passive scalar transport benchmark problems are in excellent agreement with available data. The results of Phase I effort would support a Phase II continuation.