Differential Diffusion Effects in Low Mach Number Combustion

Simulation and Analysis of Reacting Flow

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Abstract

The fidelity of flame simulations depends not only on the chemical kinetics model but also on the model used for diffusive species transport. One of the simplest is a constant Lewis number model in which the ratio of diffusion coefficients for different chemical species is assumed to be fixed. A somewhat more realistic model is to use a mixture-averaged model in which each chemical species has a diffusion coefficient that is a function of the local composition and temperature. A fully comprehensive model includes a number of additional effects including the Soret effect that represents diffusion of species along a thermal gradient, and the analogous Dufour effect that describes thermal diffusion along species gradients. In addition, a comprehensive model incorporates a full matrix of diffusion coefficients that individually specifies the diffusion of a species along gradients of all the other species. In many cases, the additional complexity of the comprehensive model is unncessary; however, for fuels that are rich in molecular hydrogen, the use of a higher-fidelity model can have a significant effect. Here we describe a new algorithm for implicit solution of the nonlinear parabolic system that describes the comprehensive transport model in the context of a low Mach number adaptive combustion algorithm. We then present numerical results illustrating the impact of transport fidelity on simulations of lean, premixed hydrogen flames.