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Simulations of Flame Acceleration and DDT in Mixture Composition Gradients[1] WEILIN ZHENG, CAROLYN KAPLAN, University of Maryland, RYAN HOUIM, University of Florida, ELAINE ORAN, University of Maryland —
Unsteady, multidimensional, fully compressible numerical simulations of methane-air in an obstructed channelwith spatial gradients in equivalence ratios have been carried to determine the effects of the gradients on flame acceleration and transition to detonation. Results for gradients perpendicular to the propagation direction were considered here. A calibrated, optimized chemical-diffusive model that reproduces correct flame and detonation properties for methane-air over a range of equivalence ratios was derived from a combination of a genetic algorithm with a Nelder-Mead optimization scheme. Inhomogeneous mixtures of methane-air resulted in slower flame acceleration and longer distance to DDT. Detonations were more likely to decouple into a flame and a shock under sharper concentration gradients. Detailed analyses of temperature and equivalence ratio illustrated that vertical gradients can greatly affect the formation of hotspots that initiate detonation by changing the strength of leading shock wave and local equivalence ratio near the base of obstacles.

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