

Abstract Submitted
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***A Priori* Analysis of Subgrid Mass Flux Vectors from Massively Parallel Direct Numerical Simulations of High Pressure H₂/O₂ Reacting Shear Layers**¹ JUSTIN FOSTER, RICHARD MILLER, Clemson University — Direct Numerical Simulations (DNS) are conducted for temporally developing reacting H₂/O₂ shear layers at an ambient pressure of 100atm. The compressible form of the governing equations are coupled with the Peng Robinson real gas equation of state and are solved using eighth order central finite differences and fourth order Runge Kutta time integration with resolutions up to $\sim 3/4$ billion grid points. The formulation includes a detailed pressure dependent kinetics mechanism having 8 species and 19 steps, detailed property models, and generalized forms of the multicomponent heat and mass diffusion vectors derived from nonequilibrium thermodynamics and fluctuation theory. The DNS is performed over a range of Reynolds numbers up to 4500 based on the free stream velocity difference and initial vorticity thickness. The results are then analyzed in an *a priori* manner to illustrate the role of the subgrid mass flux vector within the filtered form of the governing equations relevant to Large Eddy Simulations. The subgrid mass flux vector is found to be a significant term; particularly within localized regions of the flame.

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