Abstract Submitted
for the DFD16 Meeting of
The American Physical Society

Direct numerical simulations of temporally developing hydrocarbon shear flames at elevated pressure: effects of the equation of state and the unity Lewis number assumption AYSE KORUCU, RICHARD MILLER, Clemson Univ — Direct numerical simulations (DNS) of temporally developing shear flames are used to investigate both equation of state (EOS) and unity-Lewis (Le) number assumption effects in hydrocarbon flames at elevated pressure. A reduced $Kerosene/Air$ mechanism including a semi-global soot formation/oxidation model is used to study soot formation/oxidation processes in a temporarlly developing hydrocarbon shear flame operating at both atmospheric and elevated pressures for the cubic Peng-Robinson real fluid EOS. Results are compared to simulations using the ideal gas law (IGL). The results show that while the unity-Le number assumption with the IGL EOS under-predicts the flame temperature for all pressures, with the real fluid EOS it under-predicts the flame temperature for 1 and 35 atm and over-predicts the rest. The soot mass fraction, Y_s, is only under-predicted for the 1 atm flame for both IGL and real gas fluid EOS models. While Y_s is over-predicted for elevated pressures with IGL EOS, for the real gas EOS Y_s' s predictions are similar to results using a non-unity Le model derived from non-equilibrium thermodynamics and real diffusivities. Adopting the unity Le assumption is shown to cause misprediction of Y_s, the flame temperature, and the mass fractions of CO, H and OH.

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Date submitted: 30 Jul 2016 Electronic form version 1.4