1D flame problem specification

Consider a 1D premixed propane-air flame burning into room temperature (298K) reactants.

Consider the following ranges of parameters:

- pressure values of {1,10,20,30} atm,
- equivalence ratios of {0.7,0.8,0.9,1.0,1.1,1.2,1.3}.

Use the natural gas mechanism (c3_41_mech) and associated thermodynamic and transport data bases to be found at:

http://www.nuigalway.ie/chem/combust.htm#mecs

The goal is to compare solutions with different simplified/reduced mechanisms over this range of operating conditions. The choice of observable and error measure is of importance. We suggest examination of a couple of error measures. Namely

1. Laminar flame speed

2. Root Mean Square error between simplified and detailed mechanism solutions for a set of species profiles as plotted versus Temperature, specifically, we suggest the following set of species: CH3O, CH2O, C2H2, H2O2, H, O, OH, HCO, CH CO