CHEMKIN-PRO

Predicting Fuel Flexibility Impacts on Flame Speed in Burners and Boilers

Flame-speed studies are valuable aids in the design and implementation of fuel flexible burners, boilers, furnaces or incinerators. Many burner applications utilize fuels with variable composition such as syngas, landfill gas, and even variations in local natural gas composition. The flame speed behavior of one component or mixture compared to another ultimately determines key combustion characteristics such as flame propagation and flashback. CHEMKIN-PRO can quickly predict the impact of variations in fuel composition or fuel surrogate components with its laminar flame speed reactor. Flame speed is also a fundamental test of the accuracy of a fuel's chemical model (or mechanism). With an accurate chemical model, laminar flame speeds can then be predicted not only for a wide range of conditions but also for arbitrary fuel mixtures. Turbulent flame speeds are the basis for many flame-propagation models used in CFD simulations of gas turbine combustors.

Setting Up in CHEMKIN-PRO

CHEMKIN-PRO includes the Flame-Speed Calculator, which is a reactor model specifically designed to measure laminar flame speed–a fundamental property of combustion processes–and to allow parameter studies on inputs or other settings. Methane and natural gas combustion simulation in CHEMKIN-PRO uses the GRI mechanism[1]. CHEMKIN-PRO provides defaults or automated guesses for most of this parameterized study of flame speeds of methane-air mixtures at 300-700 K, equivalence ratios (phi) of 0.7-1.3 and pressures of 1-100 atm. Flame speed experiments are typically conducted at 1atm.

[1] Smith, G. P., D. M. Golden, et al. "GRI-Mech 3.0." from http://www.me.berkeley.edu/gri_mech/.
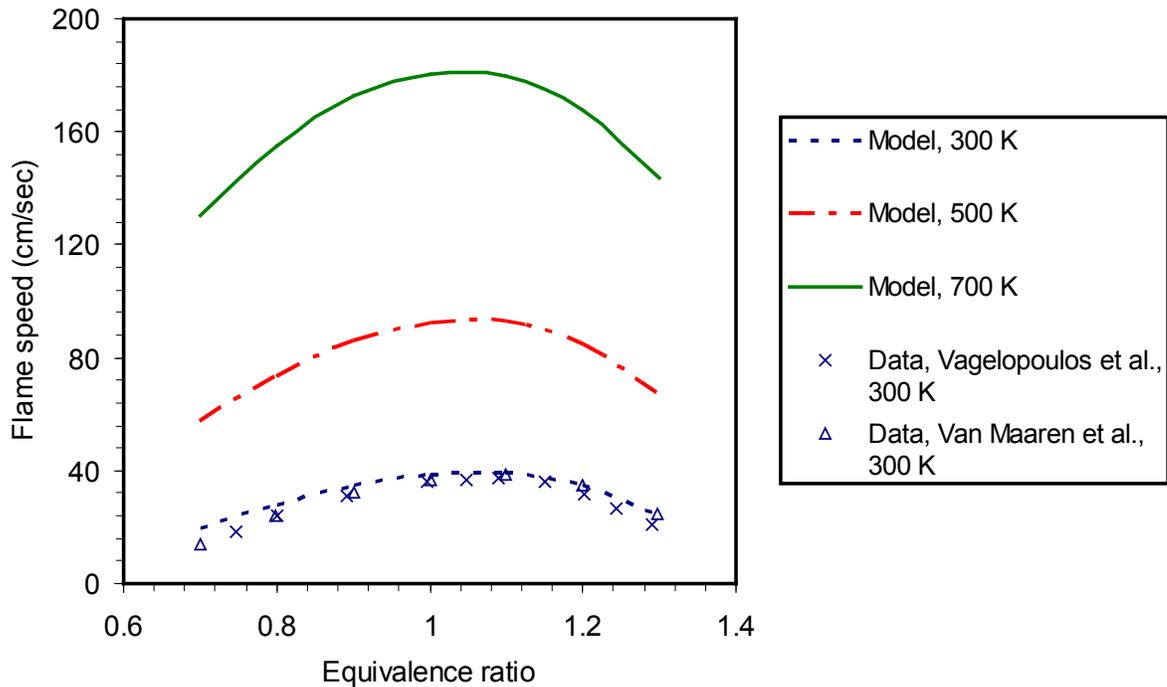
Figure 1. Calculated flame speed as a function of equivalence ratio, for unburned mixture temperatures of 300-700 K, at 1 atm, showing peak flame speeds at slightly fuel-rich conditions (equivalence ratio > 1.0).

Results

The calculated flame speeds for this simulation range from ~5 cm/sec to 180 cm/sec. The calculated flame speeds as a function of equivalence ratio and unburned gas temperatures are plotted in Figure 1. To provide a perspective on the accuracy of the calculated values, Figure 1 also shows the experimental flame speed data of Vagelopoulos et al.[2] and Van Maaren et al.[3] at 300 K. The model predictions and experimental data both show the peak flame speeds at slightly fuel-rich conditions (phi ~1.1). Studying these types of trends is valuable in understanding the kinetic and transport phenomena involved. Trends such as these can also easily be expanded to encompass other variables, such as fuel composition trends.

[2] Vagelopoulos, C. M. and F. N. Egolfopoulos. "Direct experimental determination of laminar flame speeds." Twenty-seventh Symposium (International) on Combustion, The Combustion Institute, (1998)

[3] Van Maaren, A., D. S. Thung, et al. "Measurement of flame temperature and adiabatic burning velocity of methane/air mixtures." *Combustion Science and Technology* (1994).96(4-6): 327-344.

Figure 2 shows the temperature and species profile for one case to illustrate the flame. The figure shows some of the major reactants, products and intermediates. For this case of atmospheric pressure, temperature of 300 K, and stoichiometric mixture, the flame thickness is on the order of 1 mm. The flame is centered over our domain of 10 cm, using default CHEMKIN-PRO values to ensure nearly zero gradients of gas temperature and major species at both boundaries.
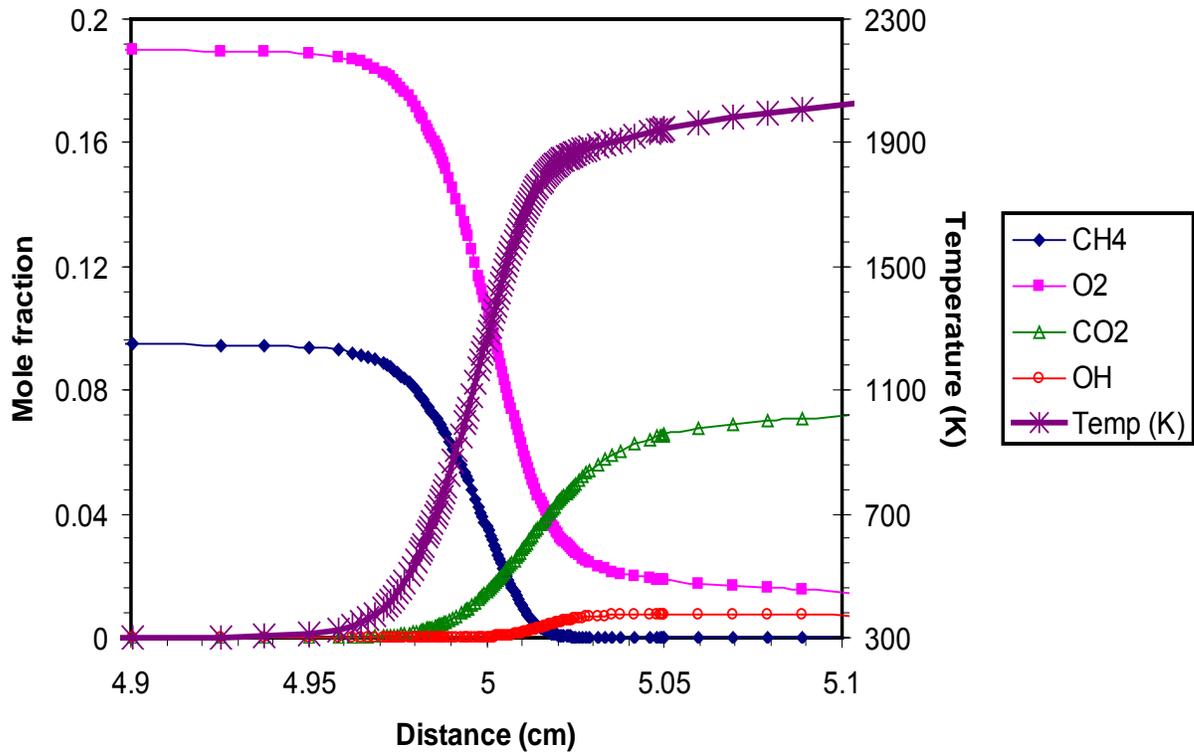
Figure 2. Species and temperature profiles for the 1 atm, 300 K, stoichiometric mixture case, showing the flame centered at 5 cm.