2.3.5 Flame Speed of Stoichiometric Methane/Air Premixed Flame

2.3.5.1 Problem description

In this tutorial we seek to determine the laminar flame speed and structure of an adiabatic, atmospheric-pressure, freely propagating, stoichiometric methane-air flame.

2.3.5.2 Problem Setup

The project file for this tutorial is called ***flame_speed__freely_propagating.ckprj*** and is located in the ***samples41*** directory. Since we are not interested in NO_x formation here, we use a skeletal methane-air combustion mechanism to speed up the calculation. As long as it contains all essential steps for methane oxidation under the desired conditions, the skeletal mechanism should yield adequate results.

For freely propagating flame problems, properties of the fresh gas mixture are entered in two different panels. Composition of the unburned methane-air mixture should be provided on the Species-specific Properties tab of the C1_Inlet1 panel and the initial guess of the mass flow rate on the Stream Properties Data tab. The unburned gas temperature, however, should be given as the first data point of the estimated temperature profile (see *Figure 2-13*). The temperature profile is located on the Reactor Physical Properties tab of C1_ Flame Speed panel (see *Figure 2-14*).

Figure 2-13 Flame Speed—Temperature Profile Panel

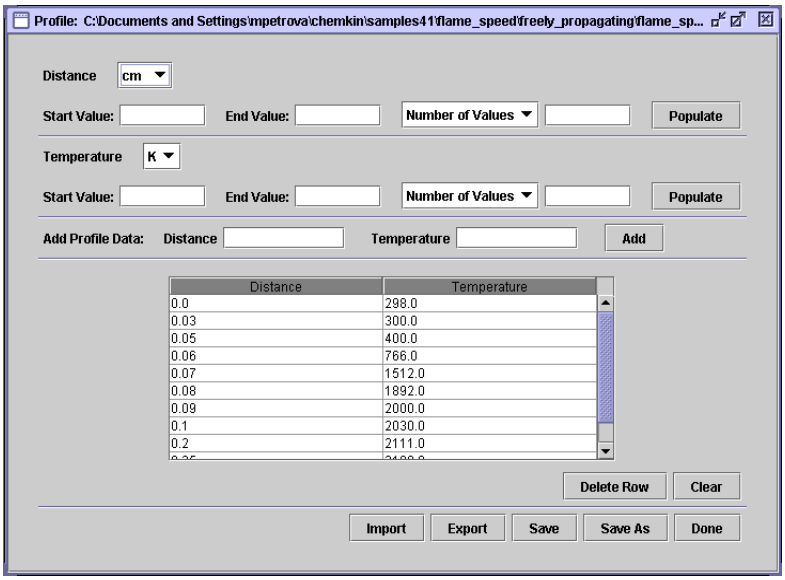
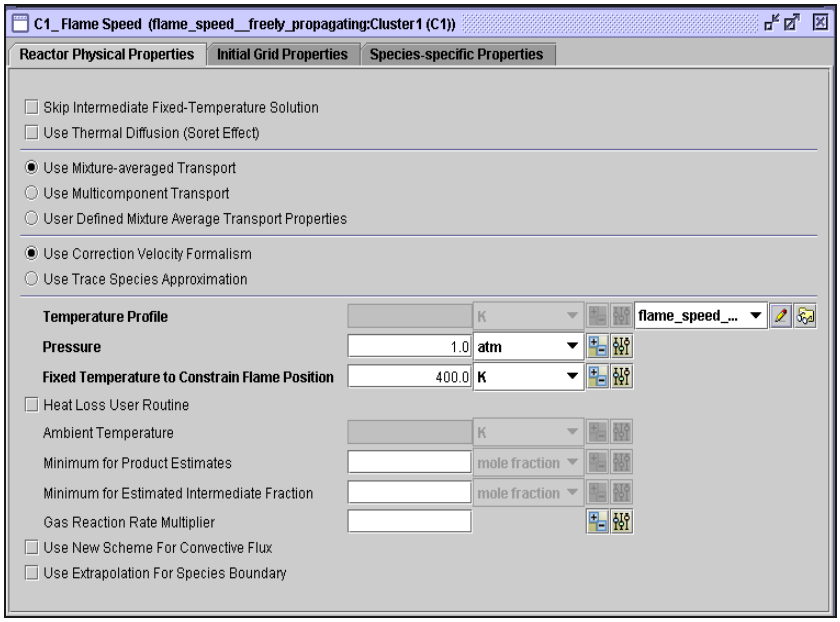


Figure 2-14 C1_ Flame Speed—Reactor Physical Property



The pressure is also entered in the corresponding field on this tab. Since the freely propagating flame problem can be difficult to solve, we follow a “proven strategy” to set up and run the problem and provide as much assistance to the numerical solver as possible to ensure a converged final solution with adequate accuracy.

First, we need to pin the flame down to establish a flame-fixed coordinate system by explicitly assigning the gas temperature at one grid point in the computational domain. The fixed temperature should be unique and must lie between the minimum and the maximum temperatures of the problem. The entry for the fixed temperature is located in the Reactor Physical Properties tab as shown in *Figure 2-14*. Initial guesses for temperature and species profiles and mass flow rate are also needed to run the problem. A good initial temperature profile is important as it can improve the convergence rate of freely propagating flame calculations. The temperature values used in the profile, except the first point, are estimates so they need not to be precise. The shape of the initial temperature profile, however, should closely resemble the actual temperature profile across the premixed flame. Since we have fixed the temperature at a point in the domain, we can easily situate the flame front and make it consistent with the guessed species profiles. The convergence rate normally is not very sensitive to the initial guess of mass flow rate but a good mass flow rate guess can be very helpful when the equivalence-ratio is close to the flammability limit. Note that the mixing zone width is larger than the initial domain. This is fine as these parameters have relatively little physical meaning, but we find that more spread-out guesses are often more likely to lead to convergence than narrow ones.

To compute an accurate flame speed, it is important to have the boundaries sufficiently far from the flame itself so that there is negligible diffusion of heat and mass through the boundary. However, we normally start with an initial run with only a few grid points and a computational domain just wide enough to encompass the flame, i.e., not necessarily the entire domain. We must make sure that a grid point corresponding to the fixed temperature is included in this initial grid, otherwise we lose the anchor of our flame-fixed coordinate system. In addition, we want to relax both gradient and curvature grid adaptation controls by setting their values close to one, meaning that relatively little mesh adaptation will be required on the first pass.

Note that the values for these two grid adaptation controls must be less than or equal to one. The solver will not perform any grid adaptation if both parameters are set to one. Once we obtain an initial solution, we will then expand the domain while reducing/tightening the gradient and curvature controls by using continuation runs (use the Continuations panel). We have to repeat this process until the temperature and species slopes at the boundaries are close to zero and both gradient and curvature controls are at least 0.5 or less.

2.3.5.3 Project Results

Solutions from the last continuation (solution number 3) are shown in *Figure 2-15* and *Figure 2-16*. The fact that the burned gas temperature of 2234 K (*Figure 2-16*) is within 3 K of the adiabatic flame temperature indicates that the final solution is an accurate one. The laminar flame speed by definition is the relative speed between the unburned gas mixture and the flame front. Since the coordinate system is fixed to the flame, all velocity solutions are actually relative velocities with respect to the flame front. Accordingly, the flame speed should be the velocity solution at the point where temperature and composition are the same as the unburned gas mixture. But, before we can conclude that velocity value is the laminar flame speed, we must check the gradients of gas temperature and major species to make sure those values are nearly zero at both boundaries. If there is any non-zero gradient at the boundaries, we will need to extend the domain farther to ensure that the assumed adiabatic and zero-diffusive-flux conditions are being maintained.

The species and temperature gradients at both boundaries are seen to be sufficiently small so there is no appreciable loss of mass or energy through the boundaries. The flame speed can be found to be 41.01 cm/sec by looking at the head of the “V” column of the last solution in the text printout. The laminar flame speed measured by Egolfopolous *et al*.[10] or the stoichiometric methane-air flame at one atmosphere is 36.53 cm/sec. The discrepancy may be due to the simplified kinetics used in the simulation or to potential non-adiabatic conditions in the experimental measurement.

Figure 2-15 Flame Speed—Axial Velocity vs. Distance

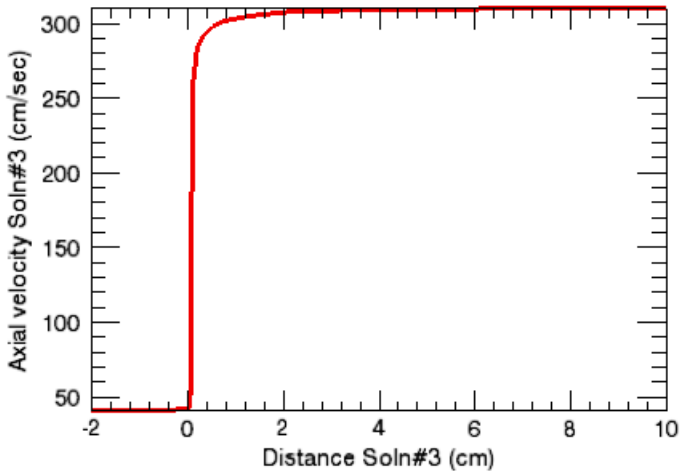
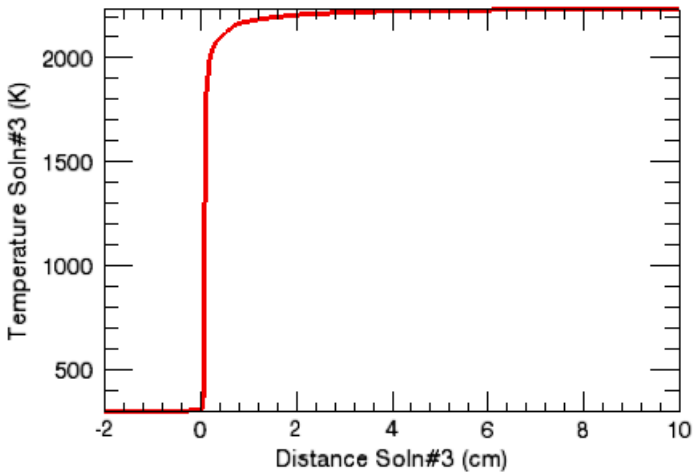


Figure 2-16 Flame Speed—Temperature vs. Distance



2.3.6 Parameter Study: Varying Equivalence Ratio of Propane/Air Flame

2.3.6.1 Project Description

This tutorial illustrates some of the features of the new Parameter Study Facility as applied to flame speed calculations of laminar, premixed flames of propane-air at atmospheric pressure. Parameter studies can be used to specify a range of values as inputs for one or more parameters. This results in several simulations being

10. F.N. Egolfopolous *et al*., *Proceedings of Combustion Institute* vol. 23 p. 471 (1988).

