Laminar Flame Speed of Stoichiometric Methane/Air Premixed Flame

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Overview

This application note describes the added features in CHEMKIN for easy setup and calculation of laminar flame speeds. We treat the example of methane-air mixtures at several pressures and equivalence ratios. This type of laminar flame-speed prediction can be used to determine the turbulent flame speed of an arbitrary gas mixture, using an empirical correlation that relates turbulent flame speeds to laminar flame speeds. Turbulent flame-speeds are the basis for many flame-propagation models used in CFD simulations of automotive engines. With an accurate kinetics model, laminar flame speeds can be predicted not only for a wide range of conditions but also for arbitrary fuel mixtures, for which experimental data might be difficult to obtain.

Introduction

CHEMKIN incorporates several additional features to the flame speed calculator model for rapid calculation setup. For this example, we use the widely known GRI mechanism[1], which is relevant for methane and natural gas combustion.

We will simulate the flame speeds of methane-air mixtures with the following conditions:

1. Initial temperatures of 300–700 K

2. Equivalence ratios of 0.7–1.3

3. Pressures of 1–100 atm

CHEMKIN provides useful defaults for several inputs as options, including an automated generation of a guess temperature profile at which to start the calculations. We will use this option, along with an initial grid based on this automated temperature profile. We will also use the default values for the solver parameters and the velocity guess value. There are several solver and initial guess input options that CHEMKIN provides for the advanced user that can be used when convergence is more difficult.

Operating-condition inputs we will provide include:

1. Un-burned gas temperature

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[1] Smith, G. P., D. M. Golden, et al. "GRI-Mech 3.0." from http://www.me.berkeley.edu/gri_mech/.

2. Value for the fuel/oxidizer equivalence ratio, and the fuel and oxidizer definition

3. Pressure

We will set up a parameter study of the above parameters to cover the range of conditions defined earlier. Using parameter studies helps in defining the whole range of conditions within a single project, and the post-processor in CHEMKIN extracts the relevant flame-speed information following the parameter study calculations. In this example, a total of 84 parameter-study cases are run to cover the range of operating conditions mentioned above.

The only grid-related inputs that we need to provide are:

1. Relative gradient and curvature parameters that determine the extent to which the solution will be refined for each case. The model uses a non-uniform grid that is successively and automatically adapted based on solution gradients determined on an initially coarse grid. The relative gradient and curvature parameters for the grid refinement are set here to a relatively tight value of 0.1.

2. Maximum number of grid points. To allow more grid points as a result of the more refined grid, we set the maximum number of grid points to 300.

3. Domain. We set the domain to be over 10 cm, to ensure that the gradients of gas temperature and major species are nearly zero at both boundaries, so that the requirement of adiabatic and zero-diffusive-flux conditions at the boundaries are met.

No other inputs need to be explicitly provided. For all other parameters we use default values that are provided in the CHEMKIN Interface.

The Flame-speed Calculator simulates a freely propagating flame, in which the point of reference is a fixed position on the flame. In this coordinate system, the flame speed is defined as the inlet velocity (velocity of unburned gas moving towards the flame) that allows the flame to stay in a fixed location, which is an eigenvalue of the solution method (see the *CHEMKIN Theory Manual* for details.) The fixed-flame coordinate system is established by explicitly constraining the gas temperature to stay at the initial fixed value at one grid point in the computational domain— this fixed temperature grid-point can either be explicitly specified by the user, or CHEMKIN can automatically calculate it.

Summary

Over the wide range of operating conditions, the model successfully converged for all 84 parameter-study cases, with no need for user intervention in the simulations beyond the initial specification of inputs described above. The calculated flame speeds vary over a range of ~5 cm/sec to 180 cm/sec. The calculated flame speeds, as a function of equivalence ratio and unburnt gas temperatures, are plotted in Figure 1. Comparisons are also made in the figure with experimental flame speed data of Vagelopoulos et al.[2] and Van Maaren et al.[3] at 300 K, to provide a perspective of the accuracy of the calculated values. The accuracy is reflective of the mechanism and the transport data used in the model. While not discussed in detail here, the results below are grid-independent; the user can ensure this for any calculation by progressively refining the grid by decreasing the values of GRAD and CURV, and observing the impact that has on the calculated flame speeds. The model predictions agree with trends in the experimental data such as the peak flame speeds typically seen at slightly fuel-rich conditions (phi ~1.1). Studying these types of trends is valuable in understanding the kinetic and transport phenomena involved. These types of trends can also easily be expanded to encompass other variables such as fuel composition trends.

Figure 1. Calculated flame speed as a function of equivalence ratio, for unburnt mixture temperatures of 300-700 K, at 1 atm

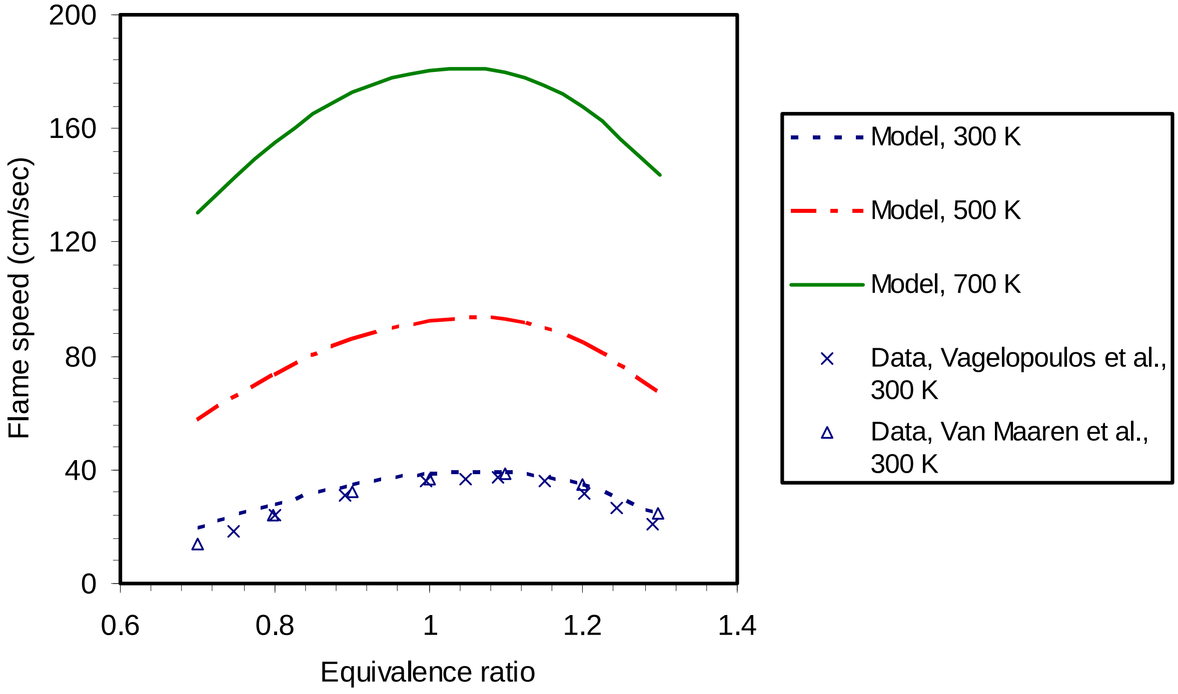

Figure 2 shows the temperature and species profile for one of the cases considered, to illustrate the flame. The figure shows some of the major reactants, products and intermediates. For this case of atmospheric pressure, temperature of 300 K, and stoichiometric mixture, the flame thickness is on the

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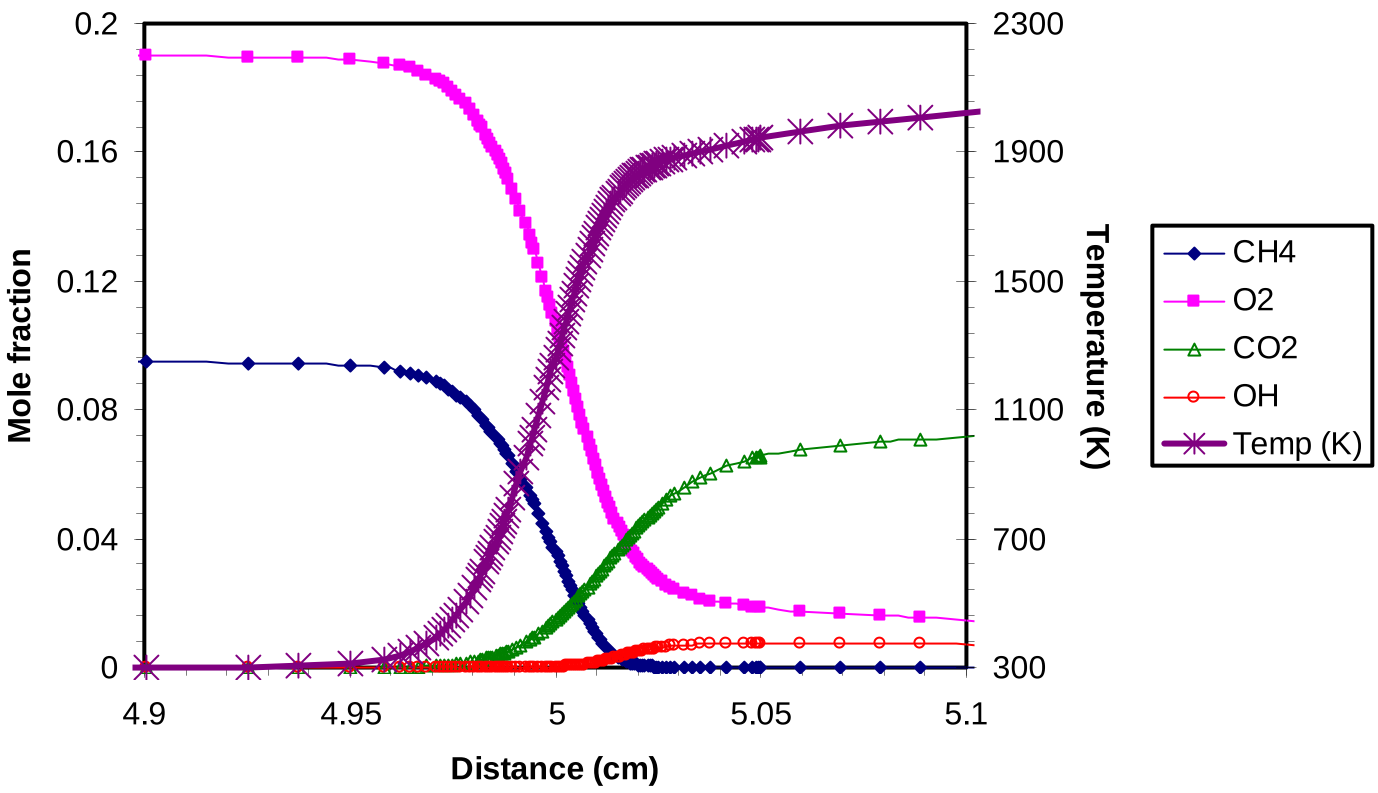
[2] Vagelopoulos, C. M. and F. N. Egolfopoulos (1998). *Direct experimental determination of laminar flame speeds.* Twenty-seventh Symposium (International) on Combustion, The Combustion Institute.

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

order of 1 mm. The flame is centered over our domain of 10 cm, using default CHEMKIN values, so that we 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



CHEMKIN allows further analysis of the chemistry effects using the Reaction Path Analyzer (see the Application Note Reaction Path Analysis).

About Reaction Design

Reaction Design helps transportation manufacturers and energy companies rapidly achieve their Clean Technology goals by automating the analysis of chemical processes via simulation and modeling solutions. Reaction Design is the exclusive developer and distributor of CHEMKIN and CHEMKIN-PRO, the *de facto* standards for modeling gas-phase and surface chemistry, providing engineers ultra-fast access to reliable answers that save time and money in the development process. Reaction Design also offers the CHEMKIN-CFD software module, which brings detailed kinetics modeling to other engineering applications, such as Computational Fluid Dynamics (CFD) programs. Reaction Design's world-class engineers, chemists and programmers have expertise that spans multi-scale engineering from the molecule to the production plant. Reaction Design serves more than 350 customers in the commercial, government and academic markets.

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