



Using the Parameter-Study Facility to Vary Equivalence Ratio in Flame-speed Calculations

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Overview

This application note illustrates some of the features of the CHEMKIN Parameter Study Facility as applied to flame-speed calculations for propane-air mixtures at atmospheric pressure.

Introduction

Parameter studies can be used to specify a range of values as inputs for one or more parameters. This results in several simulations being performed, with each run using a different specified value of the parameter, but otherwise retaining the values for other model inputs. The CHEMKIN Parameter Study Facility provides quick setup of the problem and provides 2-D or 3-D visualization of results.

Parameter studies can be used for several purposes in the context of flame-speed calculations:

- ✓ To study the impact of varying operating conditions, such as pressure, or reactant composition.
- ✓ To analyze the dependence of predictions on different values for reaction-rate parameters or transport properties.
- ✓ To test grid-independence of the solution by varying domain size or grid resolution.

The Parameter Study Facility allows several parameters to vary simultaneously. This might be useful, for instance, in reproducing a design-of-experiments matrix that varied several parameters at once.

In this example, simulations are performed with equivalence ratio as the varied parameter. Flame propagation for flames that range from fuel-lean to fuel-rich are of interest in several applications, such as engine combustion.

Project Setup

This example is set up to determine flame speeds at atmospheric pressure, using mixture-averaged transport properties. For hydrocarbon flames, the mixture-averaged approximations for diffusion coefficients, viscosity, and thermal conductivity are usually sufficient to obtain accurate flame speeds. Here we set the length of the domain to 2 cm. The reactant concentrations are specified in terms of equivalence ratio. The equivalence ratio is defined as fuel to oxidizer ratio, as compared with the stoichiometric ratio (i.e., the ratio corresponding to complete combustion to CO_2 and H_2O products). The fuel consists of pure propane, while the oxidizer is air. Since the oxidizer contains nitrogen, the stoichiometric products are CO_2 , H_2O and N_2 . Specification of these products of complete combustion

allows CHEMKIN to determine the stoichiometric ratio of fuel to oxidizer and then, with a user-specified equivalence ratio, calculate the corresponding reactant mole fractions.

To set up a parameter study, we indicate a nominal value for equivalence ratio as 1.0 and then select that parameter to vary, which gives us an opportunity to fill in a table of values. The table of values is set up by entering a start and end value for the equivalence ratio, and then selecting from one of 4 options for populating the desired distribution of values between the beginning and end value. In this example, we select 9 values to provide a range of equivalence ratios of 0.8 – 1.2.

Summary

After running the parameter studies, several plotting options are available for viewing the results as a function of the varied parameter. Some of these results are shown below.

Figure 1 shows the flame speed as a function of equivalence ratio. The flame speed is not shown as an option for single runs, since it is just one data point. However, for parameter studies, flame speed is a stored value in the solution file that can be plotted against the varied parameter.

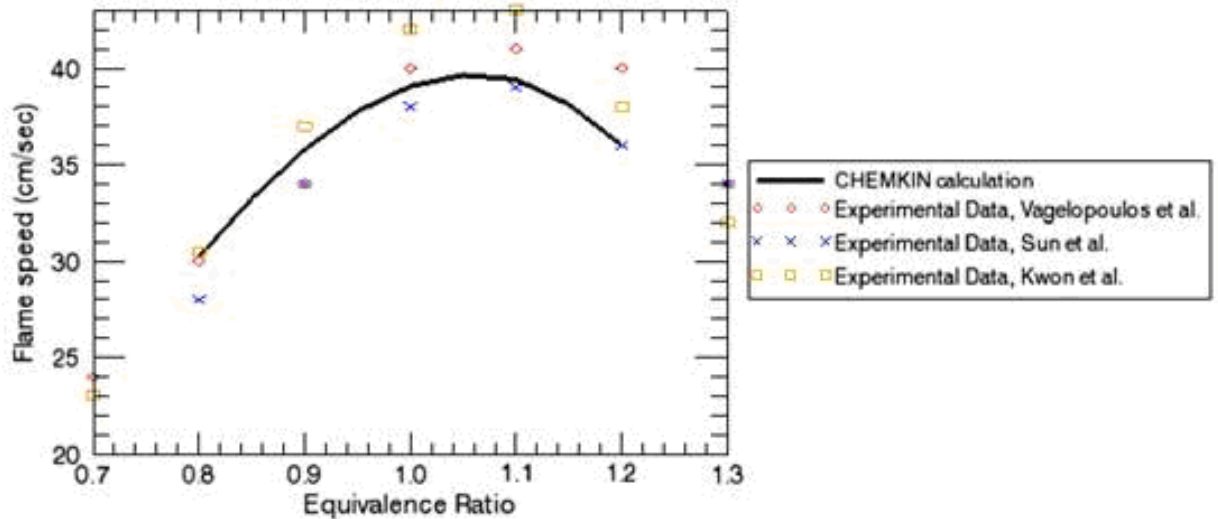
The calculated flame speeds for propane and air mixtures are compared with experimental data^{1,2,3} in Figure 1. This figure shows that the flame speed peaks at a stoichiometric ratio slightly larger than 1. In this case, the calculated values agree well with the experimental data over the range of equivalence ratios simulated, well within the spread of the experimental data. Such comparisons of flame-speed predictions against experimental data are often an important test for a combustion reaction mechanism, which tests both the kinetics and transport data for the system. In addition, for well studied fuels and validated mechanisms, such comparisons can help to test the accuracy of a new experimental set-up.

¹ C.M. Vagelopoulos and F.N. Egolfopoulos, Proc. Combust. Inst. **27** (1998) 513

² C.J. Sun, C.J. Sung, L. He and C.K. Law, Combust. Flame **118** (1999) 108.

³ S. Kwon, L.K. Tseng and G.M. Faeth, Combust. Flame **90** (1992) 230.

Figure 1. Flame Speed Calculated Values as a Function of Equivalence Ratio

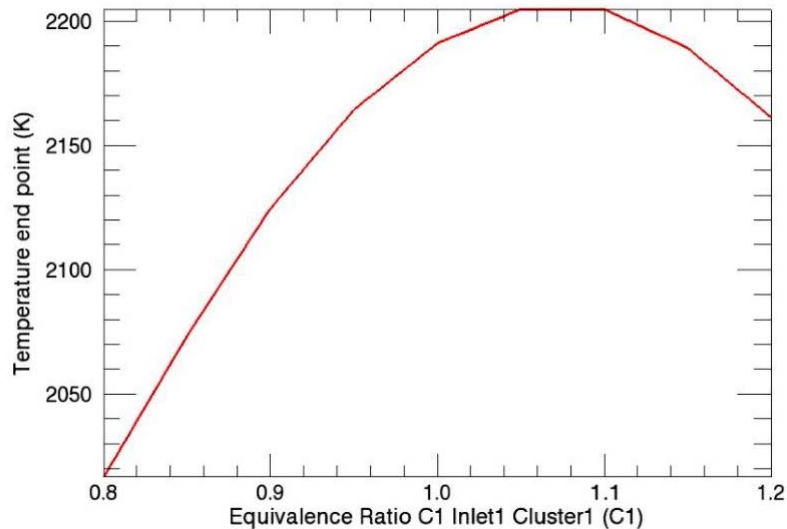


The parameter study in CHEMKIN allows you to plot values at the end of the domain for outputs such as temperature and composition, as a function of equivalence ratio. Figure 2 shows an example of flame temperature (the temperature “end point”) as a function of equivalence ratio. This type of data visualization can be helpful for other dimensional models, such as to look at the outlet concentration of a plug-flow reactor as a function of a varied parameter.

The solutions for runs 1-9 also provide detailed information on each of the individual runs, including profiles vs. distance of temperature and species, allowing visualization of the flame structure and application of reaction-path analysis on any individual flame-speed calculation (see the Reaction Path Analysis app note for more information).

Contour plots can also be made that provide 3-D visualization, showing a solution variable vs. distance (or time for transient simulations) and vs. the parameter that changes.

Figure 2. Final Temperature as a Function of Equivalence Ratio



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