



## Burner-stabilized Flame

PRO-APP-GT-1 (v1.0) May 23, 2008

### Summary

This application note presents a simulation of a burner-stabilized, laminar premixed flame of hydrogen and air at low pressure using CHEMKIN-PRO. Such flame simulations are often used to evaluate high-temperature combustion kinetics and molecular transport properties, through comparison to well controlled experiments.

### Introduction

Burner-stabilized laminar premixed flames are often used to study chemical kinetics in a combustion environment. Such flames can be modeled effectively as one-dimensional, steady-state flames, which enable detailed analysis of experimental measurements of temperature and species profiles. Examples of using flame modeling to interpret experimental observations and to verify combustion chemistry and pollution formation can be found in Miller et al.<sup>1, 2</sup>

### Project Setup

The set-up in CHEMKIN-PRO is straightforward for simulating premixed, burner-stabilized flames; we need only define the conditions at the gas inlet and the configuration of the burner.

For this case, we are using the Fixed Gas Temperature option, as opposed to solving the Energy Equation. For burner-stabilized flames, there are often significant heat losses through the burner, which may be difficult to estimate. For this reason, experimentalists usually report a measured gas temperature that can be used directly in the simulation to allow more accurate analysis of the kinetics taking place in the flame. For cases where the heat losses are known or negligible, one can solve a burner-stabilized flame problem in which the temperatures are determined from the energy conservation equation. Even if the energy equation is to be solved for the temperatures, an initial estimate of the temperature profile is required, as this is used as the starting point for the iterative solver. In any case either an estimate or the measured temperature profile must be input. For this example, only the species transport equations are solved, using the temperature as a constraint. The system pressure is 25 Torr, and Mixture-averaged Transport with the Correction Velocity Formalism are used as options for this example.

<sup>1</sup> J. A. Miller, M. C. Branch, W. J. McLean, D. W. Chandler, M. D. Smooke, and R. J. Kee, in *Proceedings of the Twentieth Symposium (International) on Combustion*, The Combustion Institute, Pittsburgh, Pennsylvania, 1985, p. 673.

<sup>2</sup> J. A. Miller, M. D. Smooke, R. M. Green, and R. J. Kee, *Combustion Science and Technology* **34**:149 (1983).

The premixed burner reactor model automatically adapts the grid during solution, starting with an initial simulation on a very coarse mesh that may have as few as five or six points. After obtaining a solution on the coarse mesh, new mesh points are added in regions where the solution or its gradients change rapidly. The initial guess for the solution on the finer mesh is obtained by interpolating the coarse mesh solution. This procedure continues until no new mesh points are needed to resolve the solution to the degree specified by the user in terms of maximum gradient and curvature for all solution variables.

In addition to the temperature profile, the simulation needs a starting estimate for the species composition profile on the initial coarse grid. This estimate is determined in terms of a reaction zone in which the reactants change from their unreacted values (the unburned composition) to the products. Intermediate species are initially estimated as having a Gaussian profile that peaks in the center of the reaction zone with the profile width such that the species fraction is  $\sim 1/10$  of its peak value at the edges of the reaction zone. The initial profiles are calculated automatically based on minimal input from the user, such as the reactant fractions. Product fractions are determined by default using an equilibrium calculation. Intermediate peak fractions may optionally be specified in cases when convergence is difficult, but such estimates are usually not necessary.

To define the gas-flow entering the burner, the inlet mass flow rate is specified as  $4.6 \text{ mg cm}^{-2}\text{sec}^{-1}$ , which corresponds to an experimental value, and the composition of the fuel-rich gas is set to 28%  $\text{H}_2$ , 9%  $\text{O}_2$  and 63% Ar.

## Summary

Figure 1 shows the experimental gas temperature profile as a function of distance imposed on the simulation. The gas composition in Figure 2 exhibits the expected behavior of the primary combustion species as a function of distance above the burner, with most of the oxygen reacting away within the first 2 cm. At the larger distances, some of the H atoms recombine to form molecular hydrogen. This would not have been important in a fuel-lean flame, but does occur in this fuel-rich situation.

Figure 1. Burner-stabilized Flame—Experimental Gas Temperature Profile

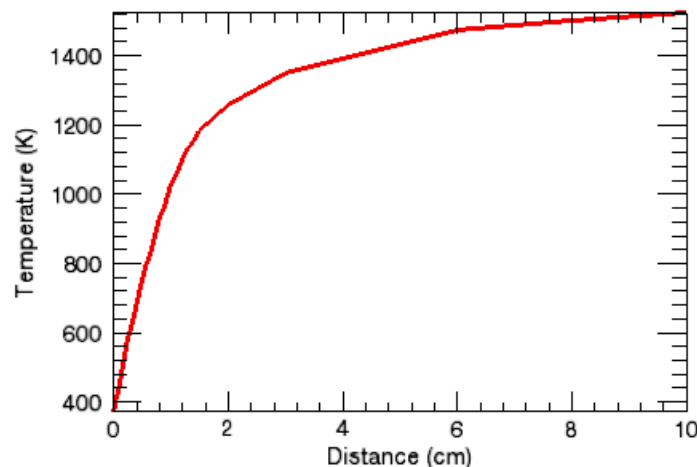
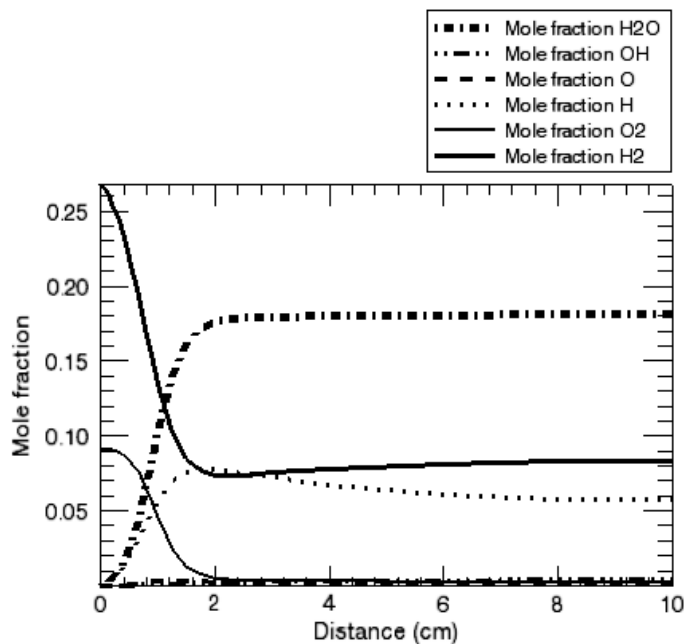


Figure 2. Burner-stabilized Flame—Mole Fractions



## About Reaction Design

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