



Flame-Extinction Strain Rate Simulations

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Summary

In this application note, the Flame-Extinction Model in CHEMKIN-PRO is used to provide calculations of the extinction strain rate for specific fuel compositions and operating conditions, under opposed-flow flame configurations. Extinction strain rate is a key combustion performance measure related to Lean Blow Off (LBO) and rich extinction in gas turbines, burners and other combustion equipment.

The Importance of Understanding the Impact of Fuels and Operating Conditions on Extinction

Flame extinction is a critical combustion performance factor in low emissions combustors, burners, rockets and many other combustion devices. The use of staged combustion, rich and lean, lowers peak flame temperatures producing less NO_x also moves the flame closer to the extinction point. Combustion parameters such as Lean Blow Off (LBO) and combustion dynamics are flame-extinction events. Fuels such as Liquefied Natural Gas (LNG) have higher concentrations of heavy hydrocarbon gaseous components, such as ethane and propane, than are present in natural gas. These higher-carbon-number gases (C₂ to C₅) can impact the extinction characteristics and produce undesirable combustion effects. Flame extinction is characterized by the operating conditions, local fuel/air ratio and the reaction chemistry of the fuel.

Flame-Extinction Model Setup

The application note describes how to use the Flame-Extinction Model in CHEMKIN-PRO to determine the extinction strain rate of a flame. Extinction analysis is conducted for a premixed stoichiometric methane-air flame at 1 atm pressure. A reduced (17 species) methane-air mechanism is used in this application.

There is a tutorial based on this application called ***opposed-flow_flame_extinction.ckprj*** located in the ***samples2010*** directory.

The stoichiometric methane-air mixture is assigned to inlet 1 (named *MethaneAir*) while pure nitrogen (N₂) is assigned to inlet 2 (named *Nitrogen*). The inlet gas temperature for both inlets is set to 296 K. The inlet velocities for both nozzles are set to 80 cm/s. Note that the first opposed-flow flame solution is thus calculated for these parameters.

The one-point option is chosen for the extinction method because a premixed fuel-air mixture is used. This choice is discussed further in the *CHEMKIN Theory Manual*. The number of extinction steps is

effectively the number of successive opposed-flow flame simulations to be conducted in search of the extinction turning point.

The nozzle velocities can be constrained for the one-point control method. In this case, we choose momentum constraint, which puts the stagnation plane roughly at the middle of the computation domain. The maximum and minimum temperature fractions are set to 0.9 and 0.5 whereas temperature steps of 10 K are used. At any point during the calculations, if the maximum temperature obtained is less than that specified by the minimum flame temperature, the calculations stop declaring that the flame existence criterion is violated. The default value of this control is 1500 K. This control is useful to avoid taking too many steps beyond the extinction point.

The input parameters maximum temperature fraction, minimum temperature fraction, and temperature step size control the location and magnitude of the internal boundary condition on temperature. The simulator first computes a nominal flame for the given input parameters. Then it finds the location at which the following statement is satisfied:

$$T = \text{maximum temperature fraction} * (\text{Current maximum temperature} - \text{Inlet temperature})$$

The temperature at this location is then successively decreased by the user-specified temperature-step-size until it reaches:

$$T = \text{minimum temperature fraction} * (\text{Current maximum temperature} - \text{Inlet temperature}).$$

A new location is then selected using the maximum temperature fraction. This process is repeated until the desired number of steps is reached or until the flame is effectively extinguished as dictated by the minimum flame temperature control.

Project Results

The output file generated by an extinction project contains the output from each opposed-flow flame simulation conducted along the path to the extinction point. The fuel and oxidizer nozzle velocities continuously increase to the value in the neighborhood of 200 cm s⁻¹. The “turning point” is reached when the MethaneAir nozzle velocity reaches about 203 cm s⁻¹. The global strain rate at the turning point is $(203 + 201)/1.4 = 289$ s⁻¹. The extinction strain rate is 550 s⁻¹.

The extinction simulator creates two raw-data output files:

opposedflow_flame_extinction_ExtingtionResponse.csv contains the data such as control temperature, pressure eigenvalue, global strain rate, “extinction” strain rate, and maximum temperature at each solution point, and

opposedflow_flame_extinction_ExtingtionProfiles.out contains the velocity and temperature profiles at each solution point with the global strain rate identifying each solution.

The file `opposed-flow_flame__extinction_ExtinctionResponse.csv` prints four strain rates. These are:

1. **KGlobal** = Global strain rate = (Fuel velocity – Oxidizer velocity) / Separation distance.
2. **KExt** = Extinction strain rate = Maximum axial velocity gradient on the fuel side just before the flame.
3. **KFuel** = Maximum strain rate on the fuel (left-hand) side.
4. **KOxid** = Maximum strain rate on the oxidizer (right-hand) side.

In these definitions, the fuel side refers to $x = 0$, i.e., left of the stagnation plane and the oxidizer side refers to $x = x_{\max}$, i.e., right side of the stagnation plane. For this premixed condition, the “fuel” side is the fuel-air mixture and the “oxidizer” side is the nitrogen gas.

The project output file can be used to get the velocity and temperature profiles at the turning point. Plotted in **Error! Reference source not found.** are the velocity and temperature profiles at extinction point obtained by using the data block for global strain rate of 289.42 s⁻¹ (use fixed-width format in Excel when loading this data block) while **Error! Reference source not found.** shows the velocity profile along with local strain rates obtained using first-order finite difference. The locations corresponding to various strain rates are also shown in **Error! Reference source not found.**

Figure 1: Flame response curve showing extinction (turning point) for premixed stoichiometric methane-air flame. The inlet temperature is 296 K and ambient pressure is 1 atm. The calculated extinction strain rate is 550 /s.

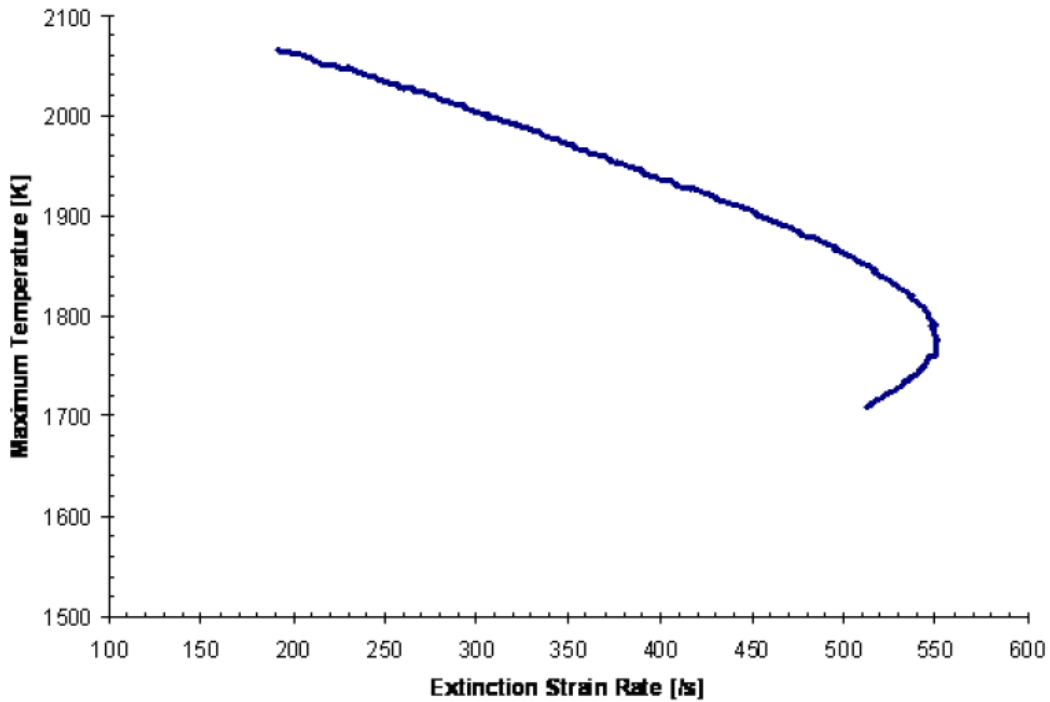


Figure 2: Axial velocity and temperature profile for premixed stoichiometric methane-air flame at extinction point. The global strain rate at extinction is 289 s⁻¹

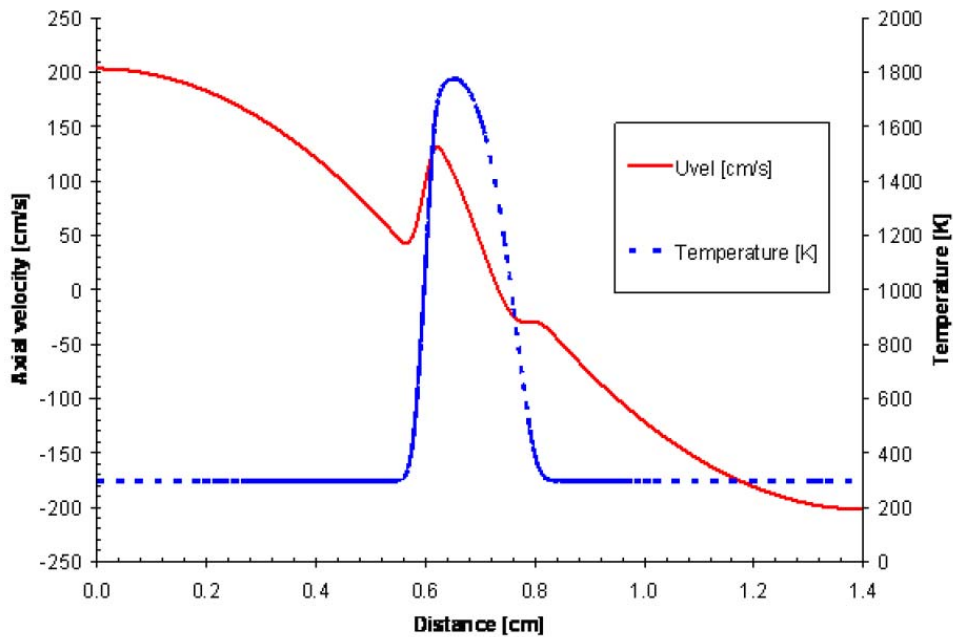
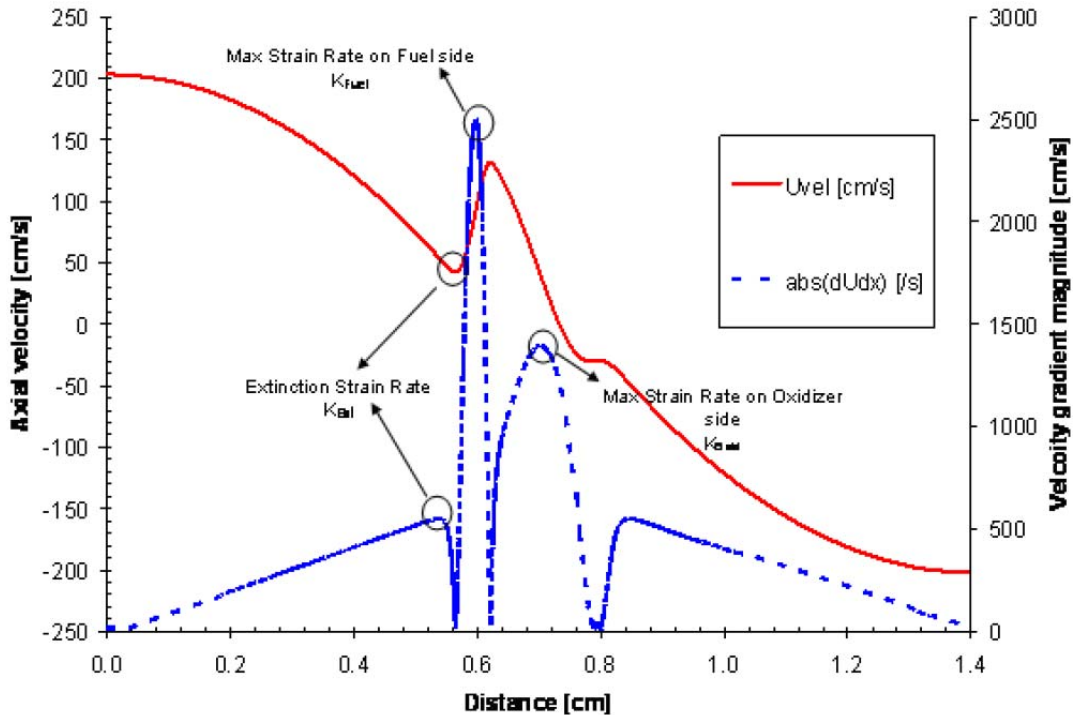


Figure 3: Axial velocity and velocity gradient magnitude for premixed stoichiometric methane-air flame at the extinction point. Also shown are the points corresponding to the definitions of various extinction strain rates



Summary

The flame-extinction model in CHEMKIN-PRO has been used to calculate the extinction strain rate for a methane-air flame at 1 atm. This model can be used to investigate the impact of key operating conditions such as pressure, temperature, fuel-air ratio and oxidizer concentration on the extinction strain rate through the use of automated parameter studies. The flame extinction model can also be used to investigate the impact of fuel composition on the extinction strain rate. These simulations are valuable in the initial conceptual design phase, during experimental testing analysis, and in diagnosing field problems.

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