Exercise 4: Flame Inhibitors

Reactor models

Solver for laminar 1D flames from the `OpenSMOKE++ Suite` [3]

Reaction mechanism

GRI-Mech 3.0[1] [4]: a) with and without a subset added for $Fe(CO)_5$ (iron pentacarbonyl) chemistry [9]; b) with and without a subset added for CF_3Br chemistry [1].

Purpose

Familiarize the student with numerical evaluation of laminar flame speeds. Introduce a practical example on the importance of chain terminating reactions.

Background

The fire suppressants currently used are largely halogenated compounds such as CF_3Br or $C_2F_4Br_2$. These halogens are now known to be harmful to the ozone layer and need to be replaced. However, it has proven difficult to find environmentally acceptable replacements. Current efforts aim to understand the inhibition mechanisms of known, effective flame inhibitors to help direct the search [9][7].

The purpose of this exercise is to investigate the effect of an inert (CO_2) and a chemically active agent (iron pentacarbonyl, $Fe(CO)_5$) on the flame speed of an atmospheric, stoichiometric methane/air flame. Employ the `OpenSMOKE_PremixedLaminarFlame1D` code to determine the flame speed, using GRI-Mech 3.0 [4]: a) with a subset for $Fe(CO)_5$ (iron pentacarbonyl) chemistry[9]; b) with and without a subset added for CF_3Br chemistry [1].

Task

1. Check the ability of GRI-Mech 3.0 [4] to correctly describe the laminar flame speed of methane in air at atmospheric pressure. For this purpose, compare the numerical calculations with experimental data reported in Figure 1.

1. Determine the amount of CO_2 addition required to obtain a 10% decrease in the flame speed of an atmospheric, stoichiometric methane/air flame.

2. Add to GRI-Mech 3.0 [4] the subset of reactions describing the chemistry of $Fe(CO)_5$ [9]. Determine the amount of $Fe(CO)_5$ addition required to obtain a 10% decrease in the flame speed of an atmospheric, stoichiometric methane/air flame. Hint: iron pentacarbonyl is much more efficient than CO2.

3. Add to GRI-Mech 3.0 [4] the subset of reactions describing the chemistry of CF_3Br [1]. Compare the efficiency of CF_3Br as fire supressant with respect to $Fe(CO)_5$. Hint: consider that 2 molecules of CF_3Br per 100 molecules of CH4 are sufficient to obtain a 10% decrease in the flame speed of an atmospheric, stoichiometric methane/air flame.

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1. The provided GRI-Mech 3.0 was simplified by removing the chemistry of NOX in order to speed-up the calculations. In the given conditions the NOX has a negligible role on the flame speed.

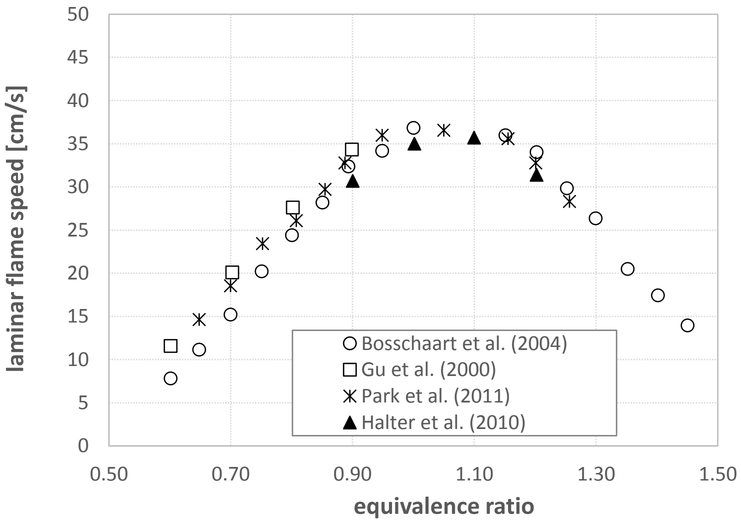

Fig. 1: Laminar flame speeds of methane/air mixtures at atmospheric pressure ($T = 298K$). Experimental data from [2, 5, 8, 6].

Procedure

Task 0: preprocessing of kinetic mechanism and thermodynamic data

Run the `OpenSMOKE_CHEMKINPreProcessor` utility on the GRI-Mech 3.0 [4] mechanism. Open the `log` file to make sure no errors were encountered in the reaction mechanism.

Task 1: comparison with experimental data

Calculate the laminar flame speed for a flame of pure methane (no additives) in air at atmospheric pressure for equivalence ratios in the range 0.7-1.3. Assume 298 K as the inlet temperature of the mixture. Use the `OpenSMOKE_PremixedLaminarFlame1D` solver on the GRI-Mech 3.0 mechanism. Compare your calculations with the experimental data reported in Figure 1.

Task 2: addition of CO_2

Calculate the amount of CO_2 which as to be added to a stoichiometric mixture of methane and air to obtain a 10% decrease in the laminar flame speed (calculated in Task 1).

Task 3: addition of $Fe(CO)_5$

- Extend the GRI-Mech 3.0 mechanism by introducing the chemistry of $Fe(CO)_5$ [9]. Remember to add not only the new reactions, but also the thermodynamic and transport properties of species involved in the new reactions.

- Calculate the amount of Fe(CO)5 which as to be added to a stoichiometric mixture of methane and air to obtain a 10% decrease in the laminar flame speed (calculated in Task 1). Hint: iron pentacarbonyl is much more efficient than CO_2, so you need only a few ppm.

Task 4: addition of CF_3Br

- Extend the GRI-Mech 3.0 mechanism by introducing the chemistry of CF_3Br [1]. Remember to add not only the new reactions, but also the thermodynamic and transport properties of species involved in the new reactions.

- Calculate the amount of CF_3Br which as to be added to a stoichiometric mixture of methane and air to obtain a 10% decrease in the laminar flame speed (calculated in Task 1). Hint: consider that 2 molecules of CF_3Br per 100 molecules of CH_4 are sufficient to obtain a 10% decrease in the flame speed of an atmospheric, stoichiometric methane/air flame.

References

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