Modeling Ignition Using One-Step Chemistry

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1 Introduction

Determining the risk of accidental ignition of flammable mixtures is a topic of tremendous importance in industry and aviation safety. The concept of minimum ignition energy (MIE) has traditionally formed the basis for studying ignition hazards of fuels. Standard test methods for determining the MIE use a capacitive spark discharge as the ignition source [1], and there have been extensive experimental studies to determine the minimum ignition energies of many different flammable mixtures. Work has been done on the numerical modeling of the hydrodynamic evolution following a spark discharge in a non-reactive gas [2]-[5] and on spark ignition in reactive mixtures using various models for the flame and spark discharge [6]-[8]. However, due to the complexity of modeling the ignition process, predicting ignition remains primarily an experimental issue.

The objective of this work is to develop a numerical model of the spark ignition process that accurately captures both the chemistry and the fluid dynamics over a range of physical scales. We use the AMROC (Adaptive Mesh Refinement in Object-Oriented C++) software package developed by R. Deiterding [9] to solve the non-reactive and reactive Euler and Navier-Stokes equations including mass diffusion with high resolution. Preliminary 2D cylindrical computations of the flow field evolving from a spark discharge in a non-reactive gas have been completed. To perform reactive simulations in an efficient manner we need to use simplified chemistry, for which we choose a one-step reaction model. We have developed methods based on thermal explosion theory for extracting physically reasonable effective activation energies and reaction orders for one-step models. We first implemented the one-step models into a steady 1D laminar flame code using Cantera software for chemically reacting flow [10] and validated the models by comparing the flame properties with those calculated using the full chemical mechanism. We then implemented our one-step model for stoichiometric hydrogen-air into the AMROC software to perform a preliminary simulation of a 1D laminar flame. The flame simulations in AMROC were validated using the flame calculations from Cantera, and the one-step model chemistry will be extended to non steady and multidimensional simulations.

2 One-Step Chemistry Model and Flame Modeling

The chemistry model used is a one-step reaction model with reaction rate

$$k = AT^m exp\left(-\frac{E_a}{RT}\right) \tag{1}$$

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where E_a is the effective activation energy for the chemical system under consideration. To extract values for the effective activation energy and effective reaction order, a method has been developed based on simple homogeneous thermal explosion theory. For a constant pressure explosion, the explosion time can be written

$$\tau_i = \frac{c_p}{q}\frac{\widetilde{R}T_0^2}{E_a}\rho^{-n+1}\frac{1}{Z}\exp\left(\frac{Ea}{\widetilde{R}T_0}\right) \quad . \tag{2}$$

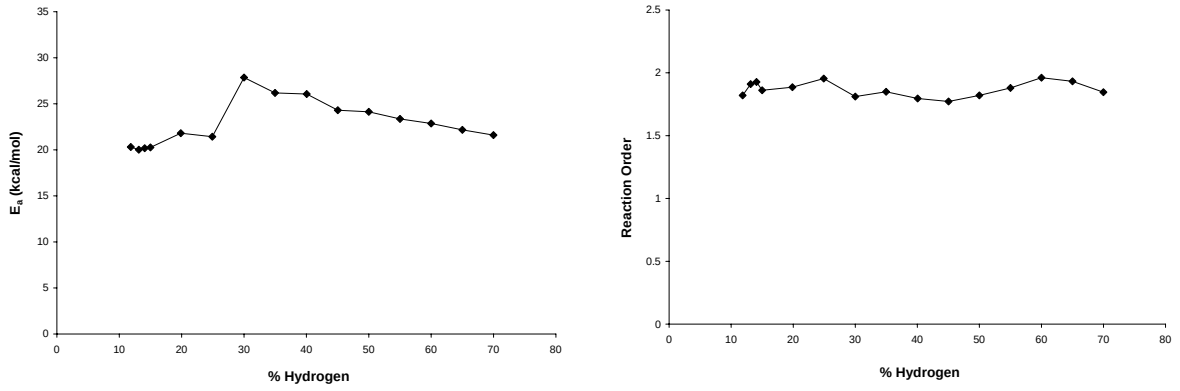
Taking derivatives of the explosion time with respect to the initial temperature, T_0, and density, ρ, while keeping the pressure and temperature constant, respectively, allows us to solve for the effective activation energy

$$E_a = \widetilde{R}T_0\left(-\frac{T_0}{\tau_i}\left(\frac{\partial\tau_i}{\partial T_0}\right)_p + (n+1)\right) \tag{3}$$

and the reaction order

$$n = -\frac{\rho}{\tau_i}\left(\frac{\partial\tau_i}{\partial\rho}\right)_{T_0} + 1 \quad . \tag{4}$$

Constant pressure explosion computations were performed with Cantera software [10] using a complex multi-step chemical mechanism [11]. The explosion times were then used to calculate effective activation energies and reaction orders for a range of hydrogen-air mixtures, as shown in Figure 1. One-step chemistry models were constructed using the computed activation energy and implemented into a Cantera 1D laminar flame code. The values of the heat release parameter, q, and pre-exponential factor, A, in the one-step model were found such that the flame speed and flame temperature matched the values calculated using a complex chemical mechanism [11]. We were able to match the flame speed and flame temperature to within 1% over the full range of compositions using the one-step chemistry models. Also, we found that a second order one-step reaction model reproduces the flame speed behavior for small changes in the initial temperature and pressure very closely, to within 6% of the complex chemistry results.



(a) (b)

Figure 1: Effective activation energies (a) and effective reaction orders (b) for a one-step model calculated using the constant pressure explosion method (Equations 3 and 4).

3 Spark Ignition Modeling

We have performed preliminary computations in AMROC to simulate the flow field resulting from a spark discharge from a conical electrode in a non-reactive perfect gas (nitrogen). The spark is modeled as a thin cylindrical region of high temperature, high pressure plasma which produces a shock wave that is spherical in nature near the electrode surface but cylindrical in nature near the vertical plane of symmetry. This shock structure leads to a complicated flow field, visualized by the evolution of the density field in Figure 2. This flow field encompasses a range of fluid dynamical scales, and will have different characteristics for different electrode geometries. Therefore, in this work we will perform fully resolved simulations to accurately capture the fluid mechanics and will investigate how different electrode geometries affect the flow field during ignition.

We will continue work on developing the one-step chemistry models by implementing them in strained flame calculations and comparing the flame behavior with calculations using the full chemical mechanism. The one-step chemistry model has been successfully implemented in AMROC for simulating 1D laminar flames and and the simulation has been validated using flame computations in Cantera. We will now implement the one-step chemistry in the 2D spark ignition simulation, allowing us to model the early stages of ignition while accurately capturing the chemistry, transport, and fluid mechanics. We will also perform simultaneous spark ignition experiments for comparison with the simulations. In the experiments the flow field following the spark discharge is visualized using high-speed schlieren optics, and the formation of the flame is tracked using PLIF imaging. These images of both the flow and the chemistry can then be used to validate the numerical simulation. By varying the spark characteristics and electrode geometry, we will examine the influence of the spark size and the flow field characteristics on flame formation.

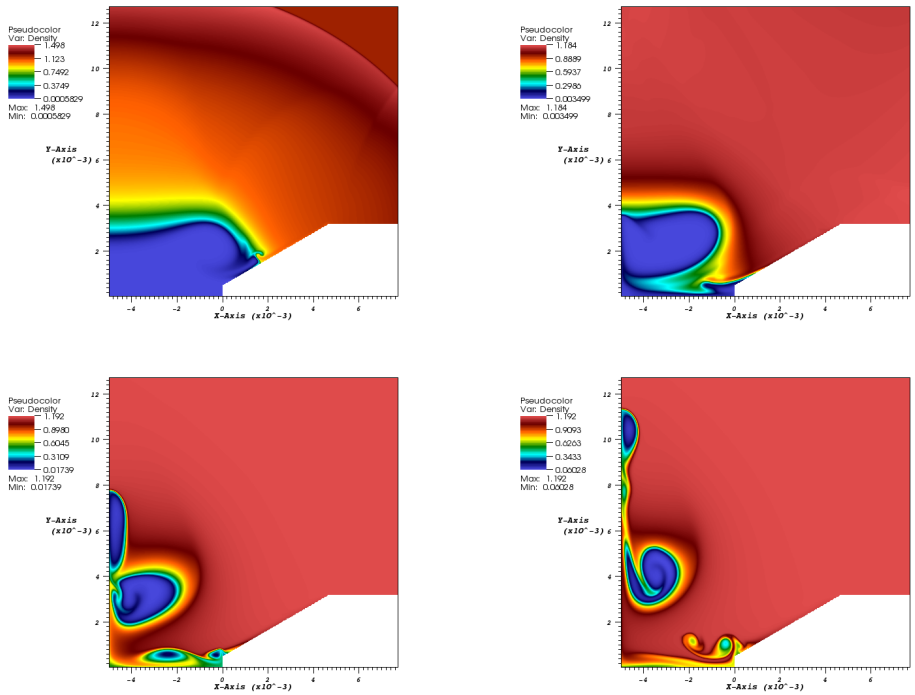


Figure 2: Evolution of the density field following spark discharge in a non-reactive gas.

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