

Modeling Hot-Surface Ignition of Hydrocarbon-Air Mixtures

S.K. Menon¹, P.A. Boettcher², B.Ventura² J.E. Shepherd², and G. Blanquart¹

*¹Department of Mechanical Engineering
California Institute of Technology, Pasadena, CA, USA*

*²Graduate Aerospace Laboratories
California Institute of Technology, Pasadena, CA, USA*

The auto-ignition mechanism of a fuel-air mixture in a low temperature, low pressure environment without a spark is not well understood. Understanding such phenomenon is important in mitigating the possibility of explosion in aircraft fuel tanks by direct contact of flammable mixture with a hot surface. This phenomenon is currently being studied using concurrent experimental and numerical approaches. The present article describes the simulation approach involving solution of the low Mach-number Navier-Stokes equations on a 2D axisymmetric structured mesh using the Immersed Boundary method to simulate the exact geometry of the glow plug. The fluid dynamics solver is coupled with detailed chemistry of n-heptane using a flamelet approach requiring solution of transport equations for the progress variable and the enthalpy. Source terms are tabulated from 1D premixed flame calculations. Results are presented for a thermal plume base flow and a single flame initiated at the glow plug. Temperature distribution and burning velocities obtained numerically are compared with experimental measurements. Simulation results are used to analyze the coupled fluid mechanics, combustion, and heat transfer driven processes responsible for the observed flame behavior. Simulations are further used to investigate variations in combustion behavior such as multiple flames and puffing behavior observed in experiments.

1 Introduction

The process of thermal ignition of a flammable mixture by a hot-surface is highly relevant to safety considerations in several areas. Previous studies have investigated these issues as pertaining to leakage of flammable gases [1], mine safety [2] and ignition of automotive and aviation fluids [3, 4]. An experimental approach is currently being pursued to investigate such effects as they relate to aircraft fuel tank safety using a setup that allows very precise control of the conditions of the flow field prior to ignition [5]. These conditions include fuel-air mixture ratio and initial temperature and pressure of the unburned gas. The motivation for this work arises from the need to provide a fundamental explanation for the coupled fluid mechanics, heat transfer and combustion phenomena leading to the experimental observations.

Analytical investigations have been pursued previously to determine the effect of hot surface conditions and orientation on thermal ignition phenomena [2]. Numerical simulations which solve boundary layer equations have been used to study the ignition of flammable mixtures by hot, moving projectiles [6], by hot, inert particles [7] and by heated vertical surfaces [8]. However, in several of these studies, a one-step reaction mechanism has been utilized to reduce computational cost and complexity of modeling full multi-step reaction chemistry.

The Flamelet Progress Variable (FPV)-level set approach formulated by Knudsen and Pitsch [9] allows multi-step reaction chemistry to be incorporated into a fluid dynamic simulation of the flow field in a computationally efficient manner. This approach helps account for the low-temperature, low-pressure reaction pathways in heavy hydrocarbon fuels which could be vital to the accurate simulation of the ignition and flame propagation process. In the present work, the solution of low-Mach number Navier-Stokes equations using the FPV-levelset approach is used to simulate a range of different conditions for which experimental data is available following which results for flame speed, structure and burning modes are compared.

This work attempts to accomplish three main objectives - understand the effect on flame propagation by heat transfer from the hot surface to the unburned gas, qualify the effect of the thermal plume on the behavior of the flame-front and investigate the variation in flame propagation observed in experiments.

The first section of the paper presents a brief discussion of the physical problems being modeled in this work. The next sections describe the governing equations, the reaction mechanism and the solution approach used to solve the coupled fluid-dynamic combustion problem. The next section describes simulation results which are compared with experimental data following which conclusions are presented and discussed.

2 Physical Problem

There are three primary physical problems associated with hot surface ignition and flame propagation that are investigated using computational methods in this work.

2.1 Development of a thermal plume

A primary effect of the hot glow plug in the experimental setup is to develop a thermal plume due to the diffusion of heat from the hot surface into the cold unburned gas mixture. The accompanying change in density results in buoyancy induced accelerating flow towards the top surface of the chamber. The upward flow produces a density, velocity and temperature gradient in the flow field prior to the ignition event. The accuracy of the simulation in predicting the propagation behavior of a flame ignited in this flow field depends directly on a realistic simulation of the thermal plume. The first task was hence, to compare flow field properties measured by experiments to the numerical simulation results prior to ignition. The primary experimental data available for this comparison was the centerline temperature profile above the glow plug obtained using an array of thermocouples suspended in the combustion chamber.

2.2 Flame Propagation

Experimental results have shown that the flame is initiated by the ignition of a kernel of hot gas right above the top surface of the glow plug. This information is utilized to artificially ignite and initiate a flame in the numerical simulations. Ignition is a complicated event involving the diffusion and convection of species and temperature in the vicinity of the glow plug. Additionally radiation

effects and surface chemistry could be potentially involved. Predicting the correct time scales for ignition beyond the scope of the current work and attention is focused on predicting post-ignition flame propagation behavior for which considerable experimental data is available for comparison. The primary data available for comparison in this case is flame location and speed under varying conditions of fuel-air equivalence ratio and pressures. Simulations are performed under matching conditions and results are compared.

2.3 Observation of unique flame behavior

Experimental results have shown unique flame behavior such as multiple flames caused by re-ignition events and flame puffing phenomena at higher equivalence ratios (>2.4) [5]. Such phenomena have been previously observed to occur in pool fires [10]. Numerical simulations are performed here which attempt to first replicate similar phenomena and then explain the processes that lead to the observed behavior.

3 Governing equations and Boundary conditions

The governing equations of fluid motion for the simulations performed here are the variable density low-Mach number Navier-Stokes equations. As mentioned previously, reaction chemistry is modeled using the combined flame progress variable (FPV) - levelset approach as formulated by Knudsen and Pitsch [9]. The FPV-levelset approach requires the solution of transport equations for additional scalar variables. The governing equations for laminar flow are presented as follows:

Mass conservation

$$\partial_t \rho + \nabla \cdot (\rho u) = 0 \quad (1)$$

Momentum conservation

$$\partial_t(\rho u) + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau + \rho g \quad (2)$$

Scalar transport equations:

Transport of progress variable

$$\partial_t(\rho C) + \nabla \cdot (\rho u C) = \nabla \cdot (\rho D \nabla C) + \dot{\omega}_C \quad (3)$$

Transport of unburned gas temperature

$$\partial_t(\rho T) + \nabla \cdot (\rho u T) = \nabla \cdot (\rho D \nabla T) \quad (4)$$

Transport of levelset

$$\partial_t(\rho G) + u \cdot (\nabla G) = \frac{\rho_u}{\rho} S_L \quad (5)$$

The transport equation for temperature relates to the unburned gas and hence it does not have any chemical source terms in it. The approach pursued here currently uses temperature in-lieu of enthalpy. Since there are no other energy loss or source terms being considered in the current simulation, the two variables (temperature and enthalpy) are equivalent. Species mass fractions,

production rates, mixture transport properties, flame speeds etc., are assumed to depend only on unburned gas temperature and the reaction progress variable. These properties are tabulated a priori using a chemical kinetic solver - FlameMaster. The numerical solver utilizes a lookup table procedure to acquire species and mixture properties during the course of the simulation.

The chamber is modeled as a sufficiently large volume. A Dirichlet boundary condition consisting of a temperature profile is assigned to the glow plug surface. The temperature at any location on the glow plug is constant in time but it varies in space along the surface of the glow plug to match experimentally determined values. The walls of the chamber are modeled as adiabatic boundaries.

4 Reaction mechanism

The experiments were carried out using two types of fuel - *n*-hexane and *n*-heptane. The simulations were carried out using a detailed chemical mechanism for heavy hydrocarbon fuels which has been extensively validated over a wide range of temperatures, pressures, and equivalence ratios [11]. Heptane was used as the fuel in all simulations since the chemistry of heptane is better understood and previous studies have shown that normal alkanes show very similar ignition and flame propagation characteristics [12, 13, 14].

5 Solution approach

The numerical simulations were performed using the NGA code [15]. The code relies on high order conservative finite difference schemes developed for the simulation of variable density turbulent flows. The symmetry of the problem allows the computation to be performed on a 2D axisymmetric structured mesh. As mentioned previously, the accurate simulation of a thermal plume originating from the glow plug in the unburned mixture is vital to predicting the propagation behavior of the flame front. A non-reacting simulation is undertaken by assigning a temperature profile to the glow plug as measured in experiments. The diffusion of heat produces a natural convection of hot gases resulting in the development of a thermal plume in steady state where the reaction progress variable globally remains at zero value. This configuration is simulated until a steady state solution is reached. This steady state solution is used as the initial value for the reacting simulation. Ignition has been observed to occur at the top surface of the glow plug in experiments. Following this observation, a kernel of hot gas is ignited *manually* using a combination of the progress variable and level set. This results in a positive value for the progress variable source term at the surface of an iso-contour defined as the flame-front following the levelset approach. The propagation speed of the flame surface and hence the iso-contour are tabulated a priori and depends on the temperature of the unburned fresh gases ahead of the flame front. The propagation speed in addition to other properties are obtained by the solver using the lookup table procedure.

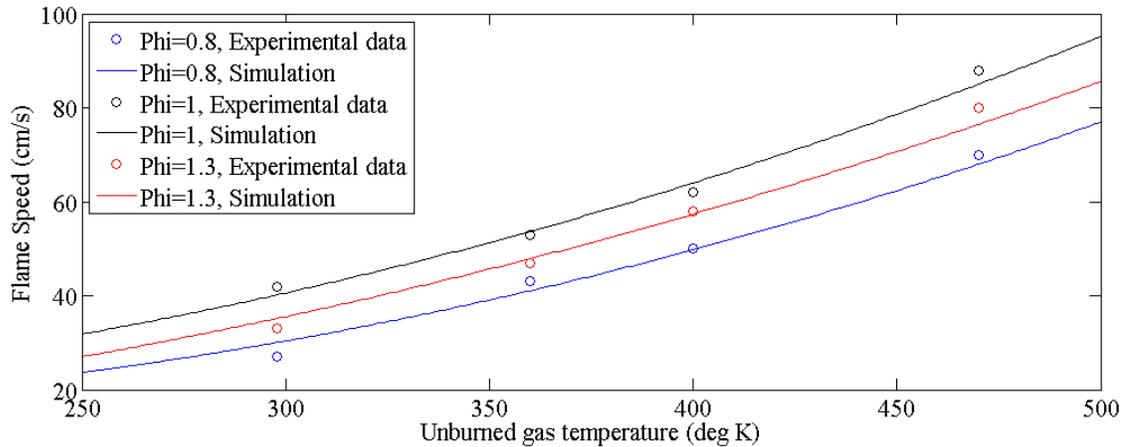


Figure 1: Comparison between laminar flame speeds calculated using n-heptane-air reaction mechanism and experimental data by Kumar [16].

6 Results and comparison

6.1 n-Heptane reaction chemistry

The reaction mechanism used in this work is used to estimate flame speeds for n-heptane-air mixtures at different equivalence ratios and unburned gas temperatures at which experimental data are available from literature [16]. The calculation is carried out using the premixed laminar flame module in FlameMaster. Figure 1 shows flame speed estimates from simulations compared to experimental results. The detailed chemical model is able to predict the effects of unburnt temperatures and equivalence ratios on the burning velocity. The agreement between simulation and experimental results shows confidence in the model and is a necessary step to run 2D fluid-flame interaction cases.

6.2 Thermal plume

Figure 2 shows the results of a 'cold' simulation where a thermal plume is stabilized over the heated glow plug. Figure 3 shows a comparison of the temperature profile above the centerline of the glow plug as obtained from the simulation and experiment. A good correlation is obtained between the two data sets.

6.3 Flame propagation

As mentioned in the solution approach, following the development of a thermal plume, a kernel of gas is artificially ignited at the top of the glow plug resulting in the development of a flame front. Figure 4 shows the results of the simulation performed for a case where the equivalence ratio (ϕ) is equal to 1. The black line in the figures represents the instantaneous position of the flame front.

The numerical simulation has been performed for different equivalence ratios and flame displace-

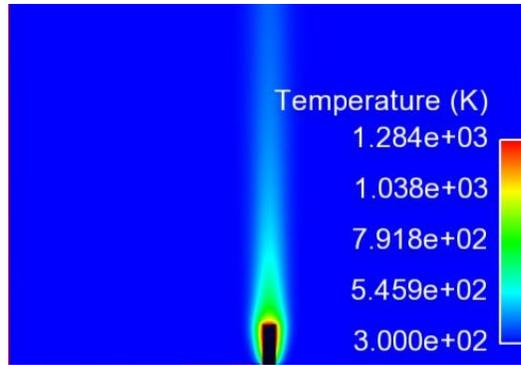


Figure 2: Simulation results for thermal plume stabilized over the glow plug at an equivalence ratio of 1.

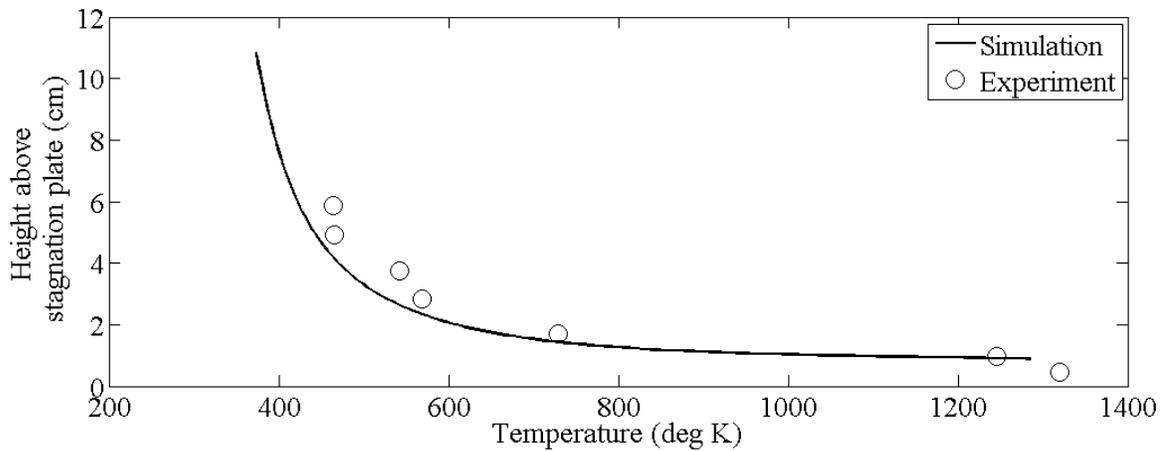


Figure 3: Comparison between simulations and experimental data for centerline temperature profile above the glow plug.

ment speeds have been estimated using simulation results. The displacement speed is defined as the absolute speed of the flame front with respect to the chamber. The effect of the thermal plume in forming a stratified temperature distribution results in considerable difference in displacement speed on the top and sides of the flame. This is also observed in the experiments. Figure 5 shows a comparison of flame displacement speeds as measured in experiments and observed in simulations. The experimental setup results in a slight difference between the displacement speed to the left and right of the flame. As seen in the figure, better agreement is obtained for the displacement speed on the sides. The simulations over-predict the displacement speed at the top for lean mixtures and under-predict the speed for rich mixtures. A considerable difference in results between simulations and experiments is seen at $\phi = 2.01$. At this equivalence ratio, an array of thermocouple elements placed above the glow plug in the experimental setup resulted in instabilities being formed at the flame front. This is believed to be the cause for the higher displacement speeds observed at this equivalence ratio. The simulations currently do not incorporate the effect of these instabilities.

An attempt was made to capture the unique flame behavior observed in experiments at rich mixture ratios. Figure 6 shows results obtained from the simulation for $\phi = 2.5$. The flame propagation

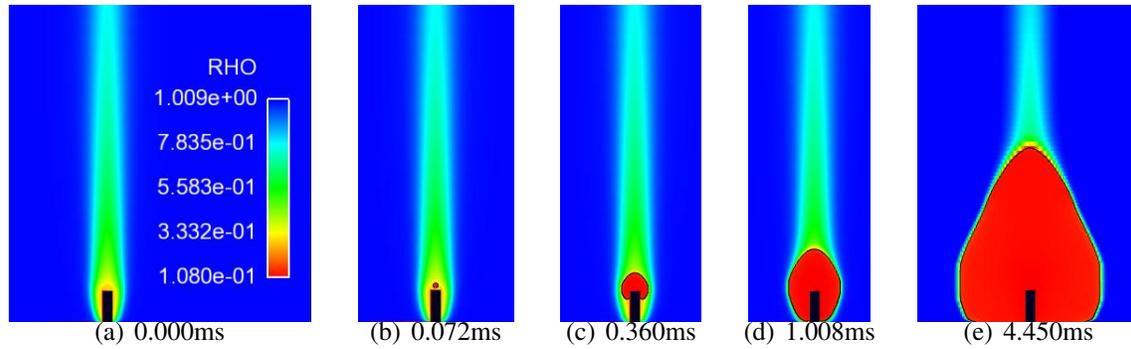


Figure 4: Simulation results for flame propagation phenomena at an equivalence ratio of 1.

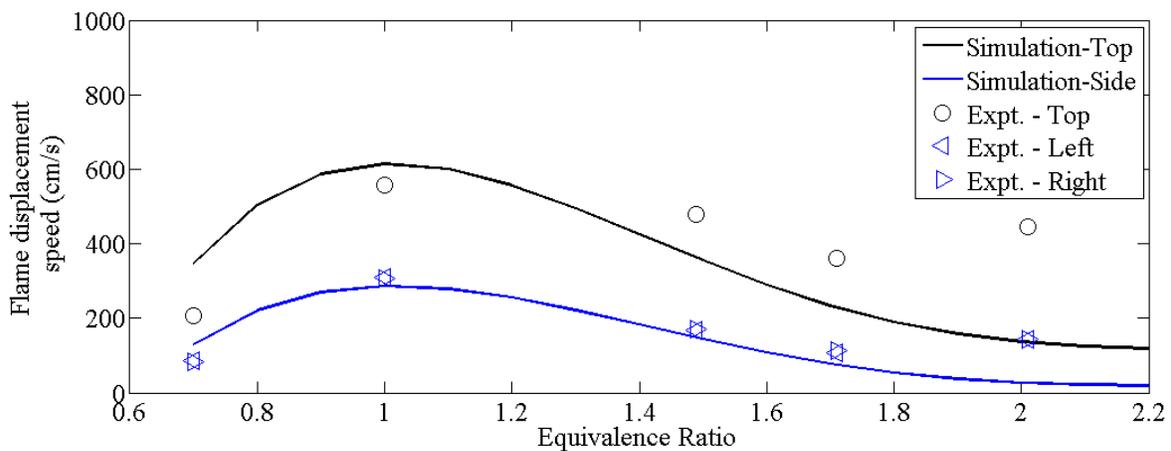


Figure 5: Comparison between simulations and experiments for flame displacement speeds at the top and bottom of the flame.

behavior is seen to be noticeably different from the case where $\phi = 1$. In this case, the flame propagates much slower at the sides than at the top. This results in the formation of an extended, narrow flame structure allowing for an entrainment region to be developed at the sides of the flame. The entrained fluid pushes up on the sides of the flame resulting in the development of flame puffs. The burned gas gradually begins to accumulate in the chamber as seen in the figure. Figure 7 shows experimental results of Schlieren images acquired for a flame propagation case with an equivalence ratio of 3 for the n-Hexane/air mixture. A marked qualitative agreement can be seen between the simulation results presented in Fig.6 and the experimental results in Fig.7. The formation of puffing structures in the flame front can be clearly distinguished in both cases. The fluid entrainment can be seen more clearly in Fig.8 where the flame structures for $\phi = 1$ and $\phi = 2.5$ are compared along with velocity vectors plotted for the flow field. Further investigation of the puffing phenomena to characterize its exact physical origin, and to compare puffing frequency and length scales with experimental results is currently underway.

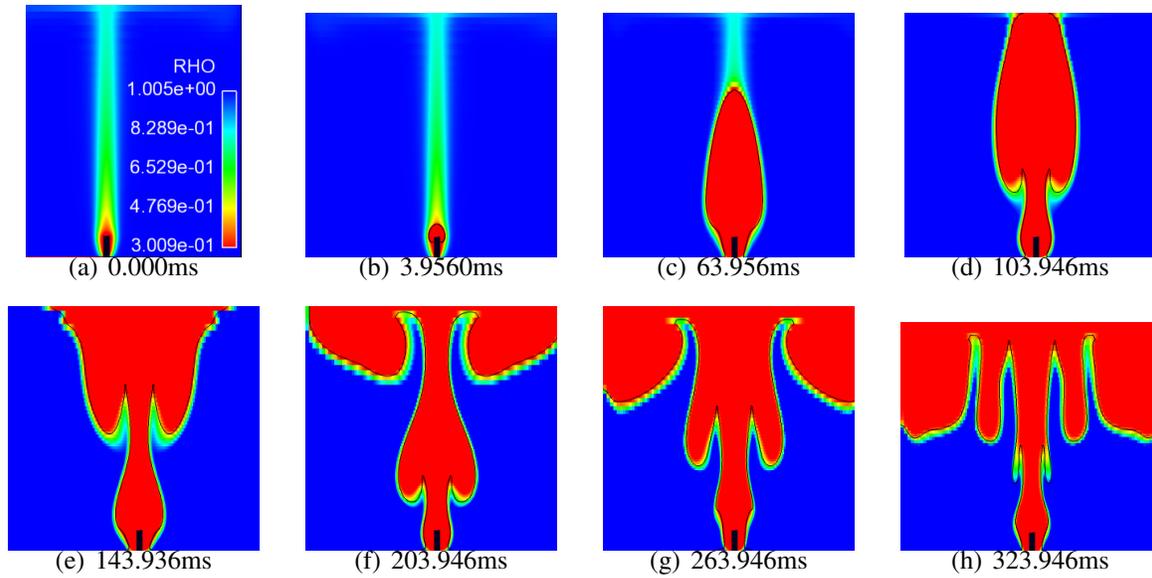


Figure 6: Simulation results for flame propagation phenomena at an equivalence ratio of 2.5.

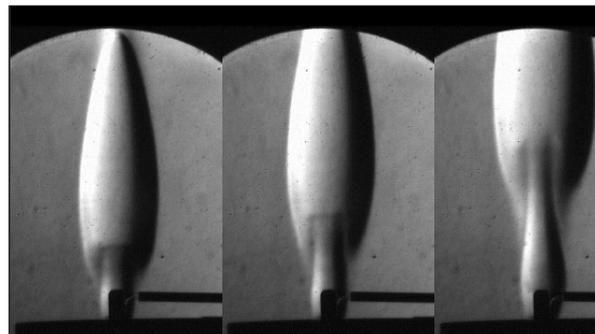


Figure 7: Schlieren visualization of flame puffing behavior for an equivalence ratio of 3.

7 Concluding Remarks

The ignition and flame propagation phenomena occurring in a flammable mixture in contact with a hot surface is studied using numerical simulations. A flamelet progress variable - level set approach is used to couple the fluid dynamic simulations with detailed reaction chemistry for n-heptane/air mixtures. The reaction mechanism is found to give good agreement for flame speed estimates with previous experimental data. The temperature profile in a thermal plume formed in the chamber prior to ignition is simulated and gives good agreement with experimental data. The simulation results for flame shape also compare well to experimental data. Flame displacement speeds predicted by simulations for the sides of the flame are found to agree well with experimental data. However, a discrepancy is seen for displacement speeds for the top surface of the flame. The flame structure is found to become narrower at high equivalence ratios similar to experimental results. Investigation of the velocity field shows the formation of an entrainment region for rich mixture ratios. Simulation results obtained for an equivalence ratio of 2.5 show evidence of puffing phenomena as

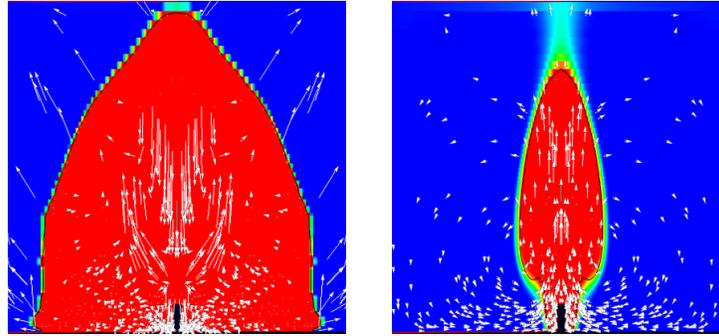


Figure 8: Simulation results for flame propagation at $\phi = 1$ and $\phi = 2.5$ shown with velocity vectors.

observed in experimental results.

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