# **Hot Surface Ignition and Flow Separation**

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# 1 Introduction

Ignition of combustible atmospheres by hot surfaces is a common issue in industrial safety. Determining critical conditions for ignition in terms of surface size and temperature are essential in order to evaluate the potential of an ignition hazard. Classical experimental work on hot surface ignition includes that of Coward and Guest [1], and Kutcha [2]. The former investigated the effect of material (e.g catalytic and non-catalytic surfaces) on ignition thresholds, whereas the latter extended this work to study the effect of variations in size and geometry. The impact of their results was hindered by their inability to measure flow velocity and composition during the ignition event. Additionally, experimental work done by Boettcher [3] using a glow plug, found the ignition temperature for n-Hexane to be essentially insensitive to composition away from flammability limits. Analytical studies have been performed by Gray [4] who investigated the effect of surface to volume ratio, and more recently that of Laurendeau [5] in which a simple model is proposed to estimate the minimum ignition temperature. Some numerical efforts in this area are due to Kumar [6] who developed a one-dimensional model to study hydrogen ignition, and the two-dimensional steady simulations of Adler [7] in which the problem of a circular hot spot in contact with reactive mixture was analyzed. Also, Boettcher [3], focused on capturing lower flammability limits with tabulated chemistry, and studying the effect of hot surface area on ignition temperature. None of the previous work has been concerned with analyzing in detail the flow field in the vicinity of the hot surface.

Simulation of hot surface ignition is challenging due to the wide range of temporal and spatial scales involved, as well as the size of detailed chemical kinetic mechanisms - large hydrocarbon fuels conventionally used in industry comprise, typically, thousands of reactions and hundreds of species. For an accurate prediction, it is thus necessary to solve the conservation equations together with transport of chemical species on a mesh small enough to capture the thermal and hydrodynamic boundary layer surrounding the hot surface. Therefore, to make the problem computationally tractable, a detailed numerical simulation of the transient viscous flow and ignition of combustible atmospheres using simplified chemistry is presented. Special attention is given to the near-wall buoyancy flow induced, and flow separation to gain insight on the dynamics, time and location of the ignition event.

## 2 Physical Model

The ignition problem is governed by the reactive Navier-Stokes equations with temperature dependent transport properties

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{1}$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \nabla \cdot \tau + \rho \mathbf{g}$$
<sup>(2)</sup>

$$\frac{\partial(\rho h)}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) = \nabla \cdot (\kappa/c_p \nabla h) + q_{chem} \Omega_R \tag{3}$$

with 
$$p = \rho \bar{R}T$$
,  $\tau = (p + \frac{2}{3}\mu \nabla \cdot \mathbf{u})\mathbf{I} + \mu[\nabla \mathbf{u} + (\nabla \mathbf{u})^T]$  (4)

The Sutherland Law, the Eucken Relation and the JANAF polynomials are used to account for the functional temperature dependence of mixture viscosity ( $\mu$ ), thermal conductivity ( $\kappa$ ) and specific heat ( $c_p$ ) respectively. The chemistry is modeled using an irreversible one-step scheme ( $R \rightarrow P$ ) in which the kinetic parameters are fitted to match the ignition delay times of the updated Ramirez's detailed mechanism [8] at  $p_o = 101$  kPa and equivalence ratio  $\Phi = 0.9$  for 900 K < T < 1600 K. Using subscript R for reactants, species mass conservation can then be written as:

$$\frac{\partial(\rho Y_R)}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_R) = \nabla \cdot (\rho D_R \nabla Y_R) + \Omega_R \text{ with } \Omega_R = -\rho Y_R A T^b \exp\left(-E/R_u T\right)$$
(5)

where  $\rho$  is density, **u** is the velocity vector, p is pressure, h is the mixture enthalpy, g is the gravitational acceleration,  $q_{chem}$  is the stored chemical energy,  $Y_R$  is the mass fraction of reactants, A is the preexponential factor, b is the temperature exponent in the modified Arrhenius rate law, E is the activation energy, and  $R_u$  and  $\bar{R}$  are the universal and specific gas constants respectively. The Lewis number is assumed to be unity which results in  $\kappa/c_p = \rho D_R$ , hence, the dynamic thermal diffusivity of reactants is used to model its mass diffusivity.

## **3** Numerical approach and simulation parameters

The equations above are integrated in two dimensions using the Open source Field Operation And Manipulation (OpenFOAM) toolbox [9]. The spatial discretization of the solution domain is done using Finite Volumes, and the pressure-velocity coupling is achieved using the PIMPLE (PISO+SIMPLE) algorithm. The geometry simulated corresponds to that used in [3], a combustion vessel of 11.4cm x 17.1cm with a glowplug of 9.3mm x 5.1mm located in the center. Figure 1 shows a schematic of the vessel together with a close up of the mesh in the vicinity of the glow plug. There are approximately 200k cells in the computational domain, compressed near the wall of the glow plug, with a minimum cell size of 80  $\mu$ m to allow for enough resolution to resolve the thermal and hydrodynamic boundary layer. Initial conditions are  $p_o = 101$  kPa,  $T_o = 300$  K,  $U_o = 0$  m/s, and  $Y_{Ro} = 1$ , with non-slip and adiabatic boundary condition on vessel walls, and a prescribed temperature ramp on the surface of the glowplug given by  $T(t) = T_o + rt$  with r = 220 K/s as in [3]. The chemical kinetics parameters used for modeling a slightly lean ( $\Phi = 0.9$ ) n-Hexane-air mixture are  $q_{chem} = 2.461 \times 10^6$  J/kg, E = 148,000 J/mol, A = 0.1618 s<sup>-1</sup> K<sup>-2.989</sup> and b = 2.989.

## 4 Results

In the present work numerical simulation of ignition by a rapidly heated surface is performed. Particularly, one of the observations made by Boettcher in [3] requires further study. According to his experiments, of 34 tests run to capture the ignition location, in 18 of them ignition was observed to

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Figure 1: Computational domain. Left: vessel geometry. Right: close-up of mesh in the vicinity of the glow plug.

occur at the top of the glowplug. In the remaining 16, ignition was reported to have taken place either on the side of the hot surface, or in the thermal plume that develops as a consequence of the buoyancy driven flow induced; why is ignition more likely to occur at the top? This study aims to answer this question and to understand the physics driving this behavior.

The simulation is initialized with the combustion vessel completely filled with reactive mixture ( $Y_{Ro} = 1$ ), and a time dependent temperature ramp is imposed on the surface of the glowplug. The temperature maximum in the computational domain and glowplug surface temperature are monitored during the course of the numerical integration to accurately determine the time to ignition. Figure 2 shows their evolution. As early as t = 4.15 s a weak departure from the prescribed temperature ramp is observed which signals the start of significant heat release taking place away from the surface of the glowplug. At t = 4.2125 s the main heat release event occurs with temperature peaking slightly over  $\sim 2500$  K and subsequently relaxing to  $\sim 2250$  K.

Figure 3 shows velocity, product mass fraction (P) and temperature fields together with velocity vectors



Figure 2: Glowplug temperature history for a heating ramp of 220 K/min

at four instances during the simulation. At t = 4 s (top left) a fully developed thermal plume can be observed. The velocity vectors clearly show the buoyancy driven flow induced. Parcels of fresh cold gas enter the thermal boundary layer from below, heat up slowly as they travel upward in close proximity

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to the wall, once they reach the upper right/left corner of the glowplug, the flow separates creating a region at the top of the glow plug where the gas is practically at rest. The gas continues to rise to the top of the combustion vessel, is forced to turn and creates a rather complex vortical flow field, a glimpse of which can be seen on the upper region of the velocity fields. Due to the aforementioned flow separation and the nearly stagnant conditions at the top of the glowplug, preferential heat diffusion ensues, readily heating up this region and in turn triggering localized chemical activity. Note however that the temperature maximum in the domain (T = 1180 K) still corresponds to that of the glowplug surface. At t = 4.21425 s (top right) the reaction rate is strong enough at the top of the glowplug to overcome diffusive and convective losses; an internal maximum appears bringing the temperature to 1500 K, roughly  $\sim 274$  K higher than the prescribed value at the glowplug surface. A short 0.25 ms later, at t = 4.21425 s (bottom left), ignition occurs and a small flame kernel forms. The abrupt expansion pushes the flow away from the ignition center, the flame front acts like a piston accelerating the flow from 0.73 m/s to 0.93 m/s in a quarter of a millisecond. Finally, the last frame on the bottom right of Figure 3 shows the initial stages of flame propagation and further acceleration of the flame front.



Figure 3: Velocity, product mass fraction and temperature fields. Top Left: at t = 4 s - early times. Top Right: at t = 4.21425 s - shortly before ignition. Bottom Left: at t = 4.2145 s - shortly after ignition/flame kernel formation. Bottom right: at t = 4.215 s - early stages of flame propagation.

In order to unravel the complex physics taking place at the top of the glowplug, each of the terms in

the energy conservation equation is plotted along its vertical centerline (see Figure 4). The plots are taken at the same times as in Figure 3 to allow for a direct comparison. The abscissas represent the normal distance from the top surface of the glowplug, whereas the ordinates show the corresponding energy density and temperature. The solid lines are the convective and diffusive heat losses, and the chemical source term given respectively by  $h_{Convection} = -\nabla \cdot (\rho \mathbf{u}h), h_{Diffusion} = \nabla \cdot (\kappa/c_p \nabla h),$ and  $h_{Source} = q_{chem} \Omega_R$ . The dashed line is the sum of the above terms, and the dashed-dotted line is the temperature. During the initial stages of heating (top left), the energy released by the chemistry is immediately balanced by diffusion close to the wall, and no contributions are due to convection providing a clear argument that the gas is effectively at rest. Away from the wall however, convection balances diffusion and the temperature is too low for chemistry to take place. As noted above, the temperature maximum remains at the wall. At t = 4.21425 s the balance is disrupted, and the sum is greater than zero up to 2 mm away from the wall. The temperature shows an internal maximum hence the rate at which heat is diffused to the wall is not large enough to counteract the rate at which heat is released by the chemistry. The dip in the convective term is due to a slight expansion of the gas in this region. The plot at t = 4.2145 s clearly indicates that ignition occurs very close to the wall roughly 1 mm away; the structure of the ignition center and the birth of an expanding flame front is distinctly captured, and the explosive nature of the ignition event can be visualized in the 7.5 fold increase in the heat release rate occuring in 0.25 ms. Finally, the last plot (bottom right) shows the typical structure of a laminar flame, with diffusion and convection balancing each other out at the front, and at the back the source term being counteracted by the combined effect of convection and diffusion but the overall balance is positive hence the rise in temperature to that of burnt products.

# 5 Conclusion

A two-dimensional simulation of ignition over a rapidly heated surface was performed. In good agreement with experiments, ignition was observed to occur at the top of the glowplug. The ignition evolution was explained in detail by means of velocity, product mass fraction and temperature fields. Additional understanding was achieved by analyzing the individual contributions of the terms in the energy conservation equation. Close to the wall, diffusion counteracts the heat release due to the chemistry, whereas far away, convection and diffusion maintain the balance. Ignition occurs when the heat release rate is greater than the rate at which heat is diffused back to the wall. Results show the importance of flow separation in creating zones/regions that are prone to ignition. Future work will compare the ignition times/locations obtained here with those of a flat plate in which flow separation does not occur at the time and length scales considered.

# Acknowledgements

Research supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) Postdoctoral Fellowship Program

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Figure 4: Contributions of each term in energy equation and temperature along vertical centerline of the glowplug. Top Left: at t = 4 s - early times. Top Right: at t = 4.21425 s - shortly before ignition. Bottom Left: at t = 4.2145 s - shortly after ignition/flame kernel formation. Bottom right: at t = 4.215 s - early stages of flame propagation.

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