# Ignition of *n*-Hexane-Air Mixtures by Moving Hot Spheres

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## 1 Introduction

Assessing the risk of accidental ignition of flammable mixtures is an issue of importance in industry and aviation. In aircraft, potential ignition sources include lightning strikes, sparks from electrical equipment, electrostatic discharge in fuel tanks, and overheated pumps. In the case of a lightning strike, hot particles are often ejected from the surface that is struck. Such hot particles represent a potential ignition hazard if they are ejected into the flammable vapor space of a fuel tank. Fuel tank makers employ multiple design techniques to prevent or contain such showers, even though there is still much that is unknown about the threshold conditions for hot particle ignition. Quantifying the ignition hazard as a function of particle material, temperature, size and velocity is a key issue for both engineering design and safety analyses.

Previous work done on hot particle ignition includes a particle heated in a furnace and then injected into an explosive atmosphere, as well as a stationary particle placed in an explosive atmosphere and heated via infrared laser light. The former experiment was performed by Silver [1] using two different particle materials, quartz and platinum. Varying the particle material had minimal effect on the minimum ignition temperature of three different flammable mixtures, 10% coal-gas/air mixture, 3% pentane/air mixture, and 20% hydrogen/air mixture. For a fixed gas mixture, the results suggest that the size and temperature of a particle are important factors in determining whether ignition occurs. The data indicate that as particle size is increased, the minimum temperature required for ignition is decreased. The experiments performed by Silver were done with particle speeds varying from 2-5 m/s, however the effect of particle speed was not investigated systematically. More recently, Beyer et. al [2] performed studies using inert particles suspended in an explosive atmosphere and heated via infrared laser light. The combustible mixtures of interest were pentane/air, propane/air, ethylene/air and hydrogen/air. The studies showed that the particle ignition temperature had low dependence on the mixture composition but was highly dependent on the combustible gas. The particle ignition temperature also showed strong dependence on the particle diameter. Additional work on stationary hot particle ignition via laser light has been performed by Dubaniewicz et. al [3] and Homan et. al [4]. By comparing the experimental data of Silver and Beyer for a pentane-air mixture, it appears that a moving particle will have a higher ignition temperature than a stationary particle at a fixed particle diameter. From our review of these previous efforts, it is clear that work on moving hot particles is limited and deserves further study.

In the current work, ignition of *n*-hexane-air mixtures is examined experimentally and numerically using moving hot spheres. Ignition tests are performed using titanium alloy (Ti-6Al-4V) spheres with a diameter of 4 mm and with varying particle surface temperatures. The experimental results are compared to the numerical flame propagation results.

## 2 Materials and Methods

### 2.1 Experimental setup

The ignition experiments were performed in a closed, cylindrical, stainless steel combustion vessel with a volume of approximately 22 L, shown in Fig. 1. Two parallel flanges are used to mount windows

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for visualization. Above the 22 L vessel sits a cylindrical, aluminum chamber with a volume of approximately 0.1 L, also shown in Fig. 1. The aluminum chamber is used to heat small metal spheres. The chamber has two parallel flanges that are used to mount tungsten electrodes which can be actuated linearly using pneumatic actuators, shown in Fig. 1(a). To heat a sphere, the tungsten electrodes which are connected to a 12 V Bosch car battery (CCA 850 Amps) make contact with the sphere on opposite sides. High current passes through the sphere thereby heating it. The tip of each electrode is contoured to maximize contact with the sphere to ensure minimal contact resistance and uniform heating.

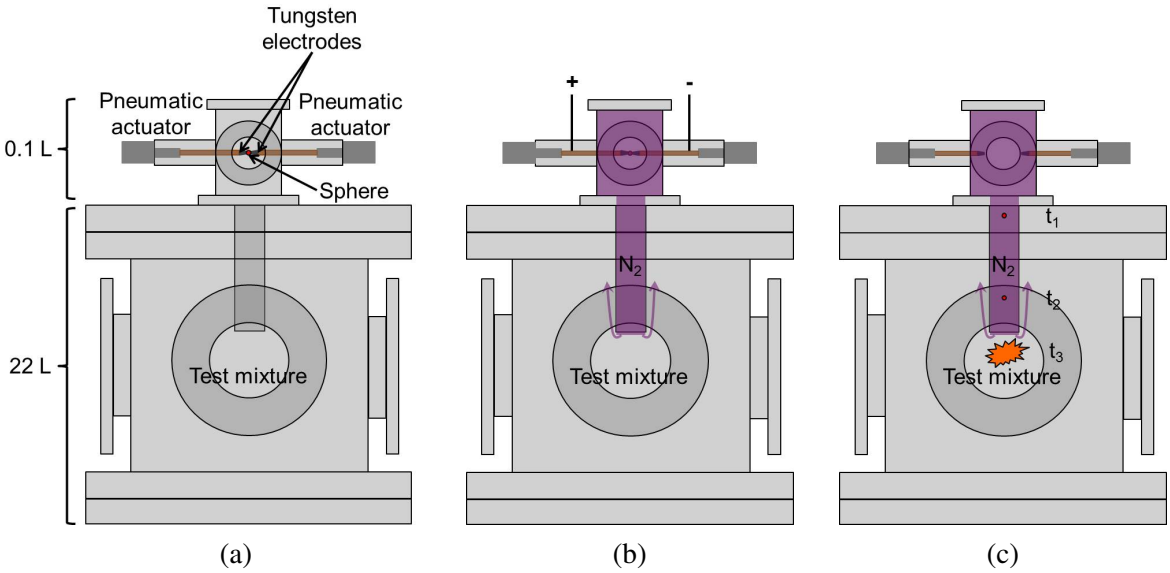



Figure 1: Experimental procedure for igniting a test mixture using a moving hot sphere.

Once a sphere is in place, a remotely controlled plumbing system is used to evacuate the combustion vessel and accurately fill it with the test mixture using the method of partial pressures, shown in Fig 1(a). A Heise manometer with a precise digital readout measures the static pressure so the gases can be filled to within 0.01 kPa of the desired gas pressure, providing precise control over the mixture composition. The aluminum chamber and a cylinder, shown in Fig. 1(b), are filled with nitrogen through a port on the chamber. This ensures that the sphere is heated in an inert environment. The free end of the cylinder is vertically aligned with the top of the combustion vessel windows. When the desired sphere surface temperature is reached, the electrodes retract allowing the sphere to fall, shown in Fig. 1(c). The sphere travels through the cylinder, containing nitrogen, then exits into the combustion vessel, containing the flammable gas mixture, coming into the field of view of the windows. A two-color pyrometer is used to measure the sphere surface temperature during heating. The temperature recorded during an ignition event and a no ignition event is the sphere surface temperature prior to electrode retraction. Three different methods were used for ignition detection. First, the pressure rise from the combustion was measured using a pressure transducer. This measurement also allowed us to determine the peak pressure rise in the vessel. Second, the temperature rise was detected using a K-type thermocouple located inside the vessel. The third method used to detect ignition was schlieren visualization of the flame propagation recorded using a high-speed camera at 10,000 frames per second.

## 2.2 Simulation setup

Numerical simulations of the experimental setup are conducted using the Flamelet Progress Variable (FPV) approach [5] which allows multi-step reaction chemistry to be incorporated into a fluid dynamic

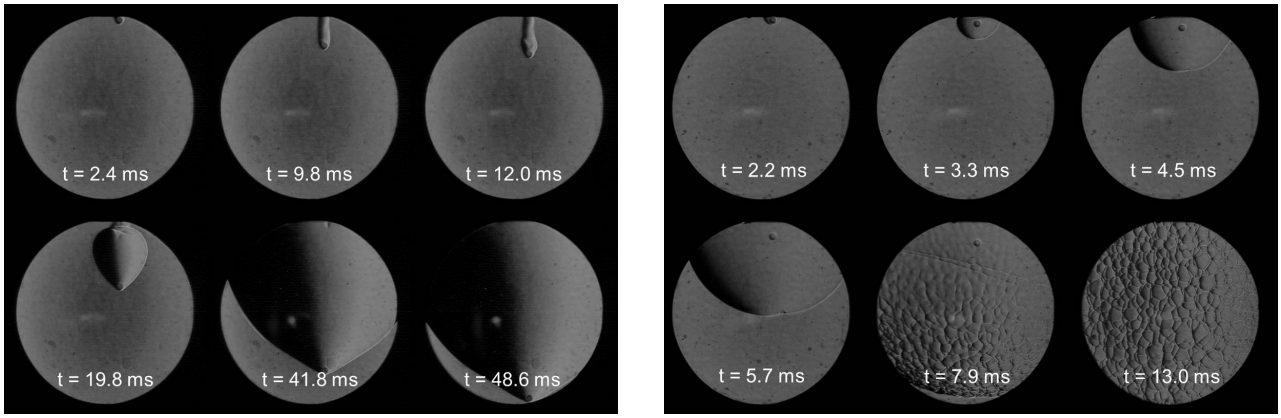
simulation in a computationally efficient manner. The governing equations of fluid motion for the simulations performed here are the variable density low-Mach number Navier-Stokes equations. The FPV approach requires the solution of transport equations for additional scalar variables. Species mass fractions, production rates, mixture transport properties etc., are computed using a chemical kinetic solver - FlameMaster [6] and tabulated a priori. The numerical solver utilizes a lookup table procedure to acquire species and mixture properties during the course of the simulation. The problem is assumed to be symmetric and simulations are carried out in a 2D axisymmetric domain corresponding to the volume of the 22 L combustion vesel. The symmetry plane established at the center-line is assigned a Neumann boundary condition. An inflow boundary condition is applied at the bottom of the chamber and a corresponding outflow condition is applied at the top of the chamber. In essence, the reacting gas mixture flows past a stationary hot sphere. The remaining surfaces except the hot sphere are modeled as closed adiabatic walls. The experimental observations indicated that the surface temperature of the hot sphere entering the flammable gas mixture is almost uniform. As a result, in the simulations, the hot sphere is initialized spatially with a uniform temperature, and remains nearly constant over the test time as indicated by the experimenal results. This Dirichlet boundary condition at the surface of the hot sphere allows for heat exchange with the surrounding fluid. The solution is obtained on a stretched non-uniform mesh consisting of 256 grid points in the vertical direction and 128 points in the radial direction. Simulations are performed using the NGA code [7]. The code relies on high order conservative finite difference schemes developed for the simulation of variable density flows. A QUICK scheme is used to compute scalar transport [8]. The experiments were carried out using *n*-hexane. 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 [9]. *n*-Heptane was used as the fuel in all the simulations since its chemistry is better understood and previous studies have shown that normal alkanes show very similar flame propagation characteristics [10, 11].

## 3 Preliminary Results

### 3.1 Overview

Ignition tests were performed for *n*-hexane-air mixtures at an initial temperature and initial pressure of 298 K and 100 kPa, respectively. The mixture equivalance ratio, $\Phi$, was fixed at 0.9 and titanium alloy (Ti-6Al-4V) spheres 4 mm in diameter were used as the ignition source. A speed of approximately 2.4 m/s was measured for each sphere using the schlieren images. Figure 2(b) shows an ignition and flame propagation using a sphere with a surface temperature of 1200 K. It is not possible to identify the ignition location using the current schlieren setup, however the time elapsed between the sphere entering the test mixture and ignition is approximately 9-10 ms. The freely propagating flame speed, 2.58 m/s [12], is within 10% of the sphere speed. The similarity in the flame speed and sphere speed is indicated by the interaction between the bottom portion of the flame and the sphere. Figure 3 shows the ignition results and probability of ignition of *n*-hexane-air at $\Phi = 0.9$ and an initial temperature and initial pressure of 298 K and 100 kPa, respectively. The probability distribution is indicated by the black line and the corresponding 95% confidence intervals are shown by the red dashed lines. The ignition results are shown by the shaded circles, where an ignition event has a probability of ignition value of 1 and a no ignition event has a probability of ignition value of 0. A narrow overlap region of 1150-1170 K exists between the ignition and no ignition results; this overlap can be attributed to uncertainty in the temperature measurements, variability in the speed of the sphere, variability in the incoming flow angle of the sphere, etc. A previous result obtained by Boettcher [13] using a stationary glow plug is also shown in Fig. 3 by the shaded triangle. The surface temperature of the stationary glow required for ignition is 910 K; using a sphere traveling at 2.4 m/s, there is 90% probability of ignition with a surface temperature of 1200 K and a 50% probability of ignition with a surface temperature of 1160 K. An additional ignition test was performed for a 40% $N_2$, *n*-hexane mixture at $\Phi = 0.9$ and an initial

temperature and initial pressure of 298 K and 50 kPa, respectively; the ignition and flame propagation are shown in Fig. 2(b). The flame propagates at 22 m/s, an order of magnitude higher than the sphere speed. In addition, the flame front becomes progressively more disturbed as it grows and exhibits significant cellular structure before the flame exists the field of view.




(a) *n*-Hexane-air ignition at 100 kPa

(b) 40% $N_2$, *n*-hexane ignition at 50 kPa

Figure 2: Schlieren images of ignition and flame propagation of *n*-hexane–$N_2$–$O_2$ mixtures at $\Phi = 0.9$ using 4 mm diameter titanium alloy (Ti-6Al-4V) spheres.

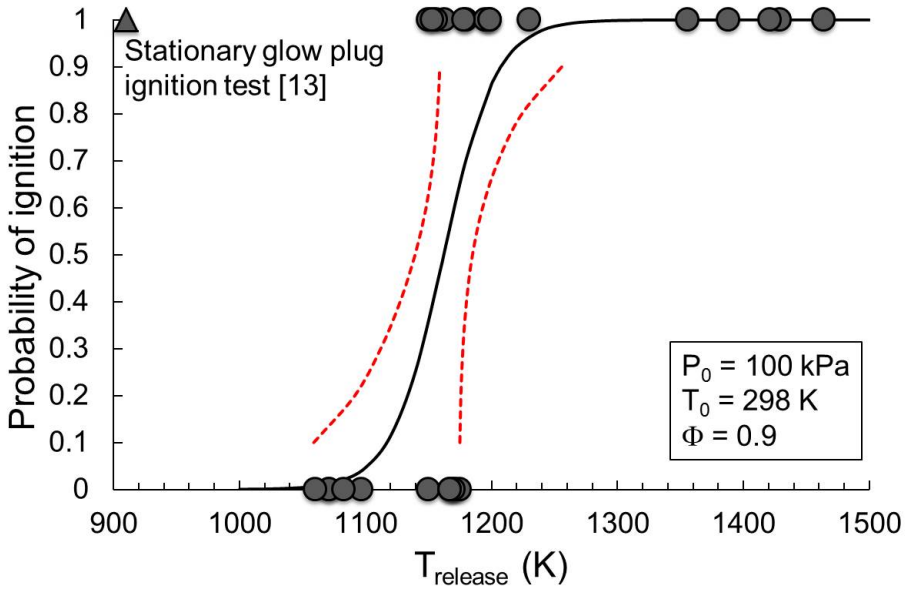



Figure 3: Ignition results of *n*-hexane-air mixtures using 4 mm diameter titanium alloy (Ti-6Al-4V) spheres traveling at approximately 2.4 m/s.

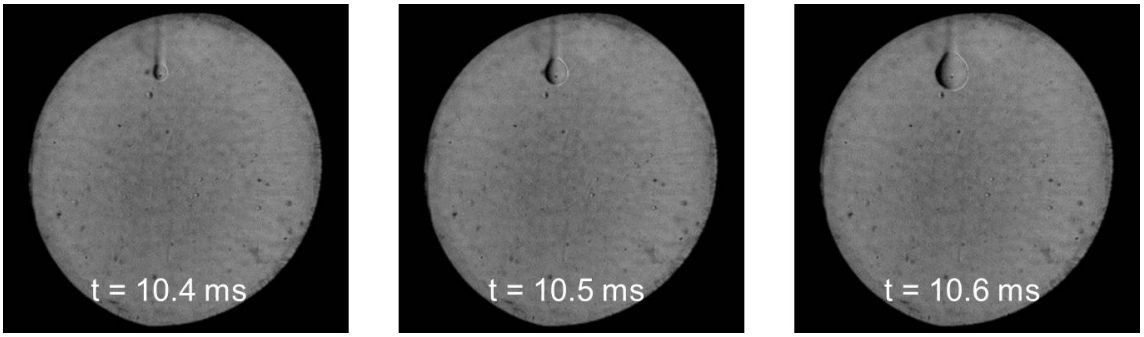
### 3.2 Hot sphere wake

As the sphere falls through the initially cold gas mixture, a boundary layer of heated gas is formed and shed from the rear of the sphere to create a wake of hot gas extending behind the sphere; this is observed in the experiment shown in Fig. 2(a). A fluid element entering the thermal boundary layer of the sphere will initially undergo a temperature rise due to diffusion of heat away from the surface. As the fluid

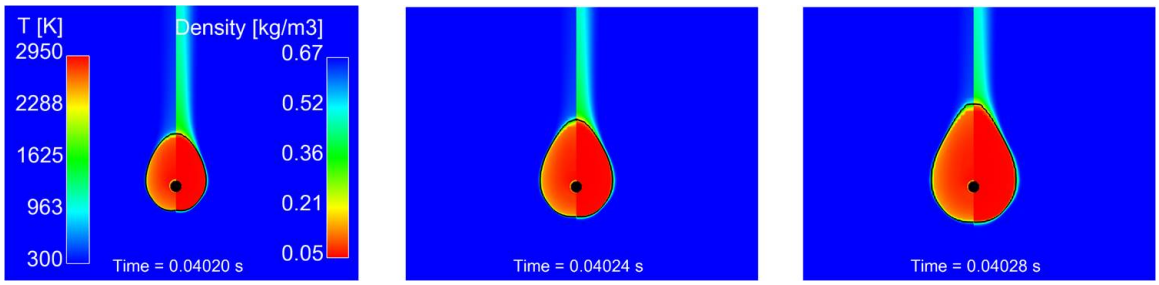
element is traveling alongside the sphere surface, there will be competing effects governing the temperature behavior: heat loss due to convection and diffusion, heat release due to chemical reactions, radical diffusion and convection. These effects ultimately lead to ignition if the sphere surface temperature is high enough.

### 3.3 Flame propagation

Shown in Fig. 4 are experimental and simulation results of a flame propagation in a 40% $N_2$, *n*-hexane mixture at $\Phi$ = 0.9 and an initial temperature and initial pressure of 298 K and 50 kPa, respectively. The particle diameter used in the simulation and experiments is approximately 1 mm and it should be noted that the particle used in the experiments is of an unknown shape. In the simulation, the ignition is assumed to take place in the wake of the sphere. The flame begins propagating radially outwards from the ignition kernel and propagates faster at the top due to the wake of hot gas extending behind the sphere, this phenomenon is observed in both the experiment and simulation. Figure 4(b) shows three images representing different time instances during the flame propagation phenomenon, the black line represents the flame front. A flame speed of 22 m/s is found for the bottom of the flame shown in Fig. 4(a). The flame speed is measured using a set of schlieren images obtained 2.6-4 ms after ignition. The time regime corresponds to a non-accelerating, stable flame. In the simulation, a flame speed of 24.5 m/s is reached at the bottom of the flame and 23.5 m/s at the sides of the flame. These values are consistent with a freely propagating flame speed of 23 m/s. The flame speed is calculated using the JetSurF [14] mechanism by multiplying the burning speed of 1.8 m/s by an expansion ratio, $\rho_u/\rho_b$, of 13; $\rho_u$ and $\rho_b$ are the densities of the unburned and burned reactants, respectively.




(a) Experimental results of flame propagation.




(b) Simulation results of flame propagation.

Figure 4: Flame propagation in 40% $N_2$, *n*-hexane mixture at $\Phi$ = 0.9 and an initial temperature and initial pressure of 298 K and 50 kPa, respectively, using a particle diameter of approximately 1 mm.

## 4 Conclusions and Future Work

In the present study, the ignition of *n*-hexane-air mixtures by moving hot spheres has been investigated experimentally. The flame propagation was observed numerically and experimentally and indicated quantitative and qualitative agreement. The experimental results indicate a narrow probability of ignition distribution for *n*-hexane-air at $\Phi = 0.9$ and an initial temperature and initial pressure of 298 K and 100 kPa, respectively. The results suggest that a sphere traveling at 2.4 m/s requires a surface temperature of 1200 K for a 90% probability of ignition which is 32% higher than the surface temperature of a stationary glow plug [13] required for ignition. A range of equivalence ratios and initial pressures will be studied to obtain varying flames speeds to understand the flame and sphere interaction in *n*-hexane-air mixtures. To further understand the effect of the added convection to the hot sphere ignition problem, the excited CH* radical will be observed in order to determine the ignition location. Future simulations will also help in determining the ignition location as well as the surface temperature required for ignition of *n*-hexane-air mixtures.

## Acknowledgements

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