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A Study of Non-Premixed Cool Flame Ignition and Extinction Subject to Unsteady Straining

As the combustion community continues to study internal combustion (IC) engines with hopes of increasing efficiency and decreasing emissions, the importance of understanding the details of the chemistry becomes ever more paramount. Certain engine technologies like homogenous charge compression ignition (HCCI) are controlled largely by the chemical processes, and under certain conditions, this type of system achieves hot ignition through a two-step process, first through low temperature and then through high temperature chemistry. Failure to fully predict such behavior leads to negative consequences, including engine knock [1].

Until only a few decades ago, high temperature chemistry was the main interest of the combustion community. This high temperature chemistry causes “hot” flames, which are those that we are all familiar with. However, more recent work has found that some fuels exhibit pronounced low temperature chemistry, with chemical mechanisms quite different from their high temperature counterparts [2]. When this low temperature chemistry is active enough, it is possible to create what are known as “cool” flames. These cool flames exhibit many similarities to hot flames, including sharp species gradients and large heat release. However, the gradients and heat release are noticeably smaller in cool flames than hot flames.

While low temperature chemistry and the relevant cool flames that it results in have been studied for decades, some difficulties have kept more advanced studies from coming to fruition. The most obvious of these is that cool flames are far weaker than hot flames, making experimental studies difficult. Due to their lower temperature, they are far less emissive than hot flames, and are therefore invisible to the naked eye [3]. Another layer of complication exists when we realize that cool flames exist as an “in between” state, separating the non-reacting, and fully reacting regions. Thus, igniting cools flames and keeping them from either extinguishing, or igniting to hot flames, comes with a large degree of difficulty. As a result, they have only been directly observed in very simple configurations under idealized conditions.

This research seeks to build upon previous work by ultimately studying non-premixed cool flames subject to unsteady straining. Firstly, I will study gaseous cool flames in the spherical non-premixed flame configuration. The basis for this work is a combustion experiment that took place on the International Space Station [4]. In this experiment, researchers burned n-heptane droplets in microgravity. Over time, the square of the diameter of the droplet decreased linearly with time as expected by combustion theory. At some non-zero diameter, the flame disappeared. However, the size of the droplet continued to decrease at a rate inconsistent with pure vaporization. Further analysis hinted strongly at the presence of a cool flame after extinction of the hot flame. Many papers have been published providing evidence for this cool flame behavior [5]. However, the spherical non-premixed cool flame has not actually been seen, and thus, has not been fully analyzed.

The difficulty in studying a steady spherical flame is that it requires low gravity or low buoyancy conditions. Microgravity is achievable on the space station, but these experiments are expensive and limited. Drop testing is a cheaper alternative, but limits experiments to a few seconds long at best. A spherical burner exists at Princeton which utilizes low pressures as well as inverted fuel/oxidizer configurations to create steady spherical diffusion flames. The goal of my research would be to use this burner to examine cool flames akin to those on the space station. While there is some experimental work in this area already, the spherical burner provides a configuration that is simpler than that on the ISS, allowing more involved study of spherical cool flames. This configuration would first be used to directly observe non-premixed spherical cool flames. Further study would involve ignition and extinction characteristics of these cool flames, with special attention placed on two-stage ignition and extinction.

Once the steady spherical cool flame has been characterized, the next step would be to study unsteady cool flames. This is difficult experimentally, so computational tools are employed.

To facilitate an understanding of unsteady cool flames, they will be studied in turbulent flow fields. This work is extremely important, as it seeks to enhance understanding of combustion physics in nearly all practical combustion devices which experience cool flames. As an example, the IC engine mentioned earlier operates under turbulent conditions. This turbulence has the potential to greatly affect the ignition and extinction characteristics of cool flames. Taking this a step forward, mistimed ignition would contribute significantly to engine knocking in an HCCI system.

My work has already taken early steps into studying the effect of turbulence on cool flames. The first step is to identify cool flames under turbulent conditions, which is facilitated by adjusting operating conditions including fuel, pressure, fuel/oxidizer temperature, and dilution, to extend the range of scalar dissipation rate over which cool flames could exist. Furthermore, consideration is given so that two-stage ignition exists, such that a non-reacting mixture first ignites to a cool flame before igniting to a hot flame as scalar dissipation rate is decreased. Additionally, the range of scalar dissipation rate between first stage ignition and second stage ignition was also maximized. Under these conditions, a two-dimensional detailed numerical simulation using a skeletal chemical mechanism is run. The simulation involves two side by side strips of diluted fuel and oxidizer in a box with fully periodic boundary conditions. Furthermore, an isotropic, turbulent-like flow field is superimposed. The results of this work will hopefully lead to an understanding of how cool flames respond to unsteady straining.

The future of this work would examine the ignition and extinction of unsteady cool flames. Both ignition and extinction have the potential to be far different due to the existence of two stage ignition and extinction. Simply put, when ignition occurs to a hot flame, the flame is in its most reactive state. That is, it cannot ignite to anything more reactive. However, when ignition occurs to a cool flame, it can still ignite to a more reactive hot flame. This can lead to conditions where the scalar dissipation rate is adjusted via turbulence such that a cool flame ignites to a hot flame, or where a nearby hot flame, through heat transfer, ignites a cool flame to a hot flame. Similarly, a hot flame that would extinguish to a non-reactive fluid may first extinguish to a cool flame, which could then proceed to extinguish again. Further work would attempt to reduce the number of simplifications present in the original simulation, and potentially even attempt to study turbulent cool flames experimentally.

[1] H.J. Curran, P. Gaffuri, W.J. Pitz, C.K. Westbrook, Combust. Flame, 114 (1998), pp. 149–177

[2] F. Battin-Leclerc, Detailed chemical kinetic models for the low-temperature combustion of hydrocarbons with application to gasoline and diesel fuel surrogates Prog Energy Combust Sci, 34 (2008), pp. 440–498

[3] Zhao, Peng, et al. "Initiation and propagation of laminar premixed cool flames." Fuel 166 (2016): 477-487.

[4] Nayagam, Vedha, et al. "Can cool flames support quasi-steady alkane droplet burning?." Combustion and Flame 159.12 (2012): 3583-3588.

[5] Farouk, Tanvir I., and Frederick L. Dryer. "Isolated n-heptane droplet combustion in microgravity:“Cool Flames”–Two-stage combustion." Combustion and Flame 161.2 (2014): 565-581.