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Ozone assisted cool flame combustion of sub-millimeter sized *n*-alkane droplets at atmospheric and higher pressure

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ABSTRACT

Cool flame combustion of individual and isolated sub-millimeter sized *n*-heptane (n-C_7H_{16}) and *n*-decane (n-$C_{10}H_{22}$) droplets are computationally investigated for atmospheric and higher operating pressure (25 atm) conditions with varying levels of ozone (O_3) mole fractions in the surroundings. A spherosymmetric, one-dimensional, transient, droplet combustion model is utilized, employing reduced versions of detailed chemical kinetic models for the fuel species and an appended ozone reaction subset. Comprehensive parametric computations show that the regime of the cool flame burning mode and the transition from cool to hot flames are sensitive to the changes of O_3 loading, pressure, diluent variation, the strength of initiation source, and the influence of fuel vapor pressure at the ambient condition. For both fuels and over a range of O_3 concentrations in the ambient, sustained cool flame burning can be directly produced, even for sub-millimeter sized droplets. Over some range of O_3 concentrations, operating pressure, and drop diameter, a self-sustaining, continuous cool flame burn can be produced without incurring a hot flame transition. For sufficiently high O_3 concentrations, combustion initiation is always followed by a hot flame transition. Fuel volatility is also shown to be important for initiation and transition to cool flame and hot flame initiation. For fuels having a flash point lower than the ambient temperature (e.g. *n*-heptane), atomic O radicals formed by O_3 decomposition react with the partially premixed, flammable gas phase near the droplet surface, leading to OH radicals, water production, and heat that auto-thermally accelerates the combustion initiation process. For fuels with flashpoints higher than the ambient temperature (e.g. *n*-decane), the reaction progress is limited by the local fuel vapor concentration and the necessity to heat the droplet surface to sufficiently high temperatures to produce locally flammable conditions. As a result, the initial transient for establishing either cool flame or hot flame transition is significantly longer for high flash point fuels. The transition of locally partially premixed reaction to diffusive burning conditions is more evident for high flash point conditions.

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1. Introduction

Observations of long-duration cool flame burning of isolated *n*-alkane droplets with a large initial diameter (D_o) under microgravity conditions [1–5] demonstrate an interesting venue for the study of diffusive cool flame burning. The term, “cool flame” has been historically associated with observations involving homogenously premixed conditions [6,7]. The cool flame diffusive burning mode of an isolated droplet is governed by a strong coupling between the low-temperature chemistry and diffusive transport that is significantly different than for premixed cool flame, static reactor or flow reactor conditions.

For hot flame isolated droplet combustion, three types of classical hot flame phenomena are observed; 1) radiative extinction; 2) diffusive extinction, or 3) complete consumption of the liquid droplet. The extinction phenomena occur at some finite liquid droplet size as the rate of heat loss to the surroundings exceeding the reaction zone heat generation. Radiative extinction occurs at larger droplet sizes as the flame radius expands upon initiation towards what would be its hypothetical stoichiometric location, to undergo extinction as the ratio of radiative heat loss to heat generation exceeds unity. For fuels that have sufficiently active low and intermediate temperature kinetic activity, the radiative extinction behavior can transition to cool flame diffusive burning. For example, in experiments aboard the International Space Station (ISS), large *n*-heptane (n-C_7H_{16}) droplets ($D_o > \sim 4$ mm) ignited in the air at atmospheric pressure the hot flame phenomena

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occurring initially radiatively transitions to a cool flame diffusive burning mode [2]. For smaller *n*-heptane droplets that do not have overwhelming radiative loss from the flame, only hot flame burning is observed, leading to diffusive extinction or complete liquid phase consumption. Hence, cool flame diffusive burning appeared to a phenomenon that could only be studied through first invoking significant radiative losses.

However, in more recent ISS experiments using *n*-decane (*n*-$C_{10}H_{22}$) droplets (D_o ~4 mm) [5], cool flame behavior was able to be achieved directly by controlling the hot wire initiation energy–current amplitude and duration. Numerical analyses reveal that as a result of the high flashpoint of *n*-decane (319.3 K [8]), modulation of the initiation energy can be utilized to control the formation rate of partially premixed flammable fuel/air mixtures near the drop surface, and hence, control the heat release associated with vapor phase reaction. By controlling the initiation energy deposition, both direct cool flame and hot flame burning modes are achievable. The flashpoint of *n*-C_7H_{16} (269.3 K [9]) is lower than the ambient air temperature in ISS experiments (298 K), and significant volumes of flammable fuel/air vapor mixture are readily formed during the droplet growth and deployment phase prior to application of hot wire initiation energy. The total ignition energy available is strongly influenced by the available partially premixed flammable mixture near the drop surface, and thus controlling hot wire initiation energy is ineffective in controlling the applied ignition energy. The overall ignition energy dependence on fuel flash point relative to the ambient temperature is also influenced by the initial droplet size, but cool flame droplet burning continues to be much more easily observed under ISS conditions and droplet sizes that result in the radiative extinction of large droplets.

The question remains as to whether other means might exist to control initiation energy deposition rate parameters so as to establish cool flame burning directly for small initial droplet sizes. Should this be achievable, cool flame droplet burning phenomena might not only be observed on ISS over a larger range of initial droplet sizes but perhaps even in ground-based facilities such as drop towers [10] or isolated, freely falling droplet experiments [11]. In fact, ground-based experiments might enable the use of multiple diagnostic and chemical analytical methods not possible to be implemented on ISS.

Recently in counterflow, pre-vaporized, laminar diffusion flame configurations, the addition of ozone to the oxidizer flow stream has been demonstrated as a mean of achieving stabilized cool flame burning conditions [12–14]. The rapid decomposition of O_3 produces active atomic oxygen (O), that substantially reduces the induction timescale for initiating low temperature, exothermic fuel oxidation chemistry, leading to flame initiation and quasi-stable cool flame diffusive burning at intermediate reaction temperatures characteristic of the negative temperature kinetic regime. Adoption of a similar O_3 addition approach to isolated droplet combustion configurations might achieve the goal of observing the cool flame droplet burning mode with smaller droplet size.

The primary objective of this study is to computationally evaluate the potential of O_3 addition to directly induce cool flame burning for sub-millimeter sized low and high flash point fuels, i.e. for *n*-C_7H_{16} and *n*-$C_{10}H_{22}$ droplets, respectively. We investigate two initial droplet diameters ($D_o = 0.1$ and 0.5 mm) and two ambient air pressures (1 and 25 atm) seeded with different levels of O_3. The role of fuel flash point, vapor pressure, and liquid phase thermodynamic and transport properties on cool flame initiation and burning characteristics are elucidated, including the time-dependent evolutions of the surrounding gas temperature and intermediate/product species fields. For such small droplets, over the entire combustion event leading to self-sustaining hot flame or cool flame burning, radiative heat loss transfer effects are negligible.

2. Numerical modeling

This computational study is performed using a spherosymmetric multi-component droplet combustion model developed previously, the details of which can be found elsewhere [10,15–18]. Important attributes of the model lie in its capability of incorporating detailed gas phase kinetics, multi-component transport formulation, spectrally resolved radiative heat transfer and heat transfer perturbation effect from the presence of tethering fibers.

The simulations are performed using numerically-reduced kinetic models for *n*-C_7H_{16} [19] and *n*-$C_{10}H_{22}$ [20] combustion developed previously. The *n*-C_7H_{16} and *n*-$C_{10}H_{22}$ models consist of 128 species undergoing 565 elementary reactions and 233 species undergoing 1266 elementary reactions respectively. Both models were obtained from a detailed kinetic construct for straight chain *n*-alkane combustion kinetics for carbon numbers from 7 to 16 [21,22]. The data correlations reported in Daubert and Danner [23] are used in evaluating liquid phase properties.

The coupled set of partial differential and algebraic equations are discretized in two steps- first in space and then integrated temporally as a set of coupled ordinary differential-algebraic equations. A node-centered finite volume approach with second order accuracy is employed for spatial discretization. The interface between the gas and liquid phases outlines the volume boundaries. The inner zone corresponds to the liquid phase fuel while the outer zone represents the gas phase ambient including the far-field which is defined as two hundred times the initial droplet diameter. Prescribed fixed ambient composition and temperature are constrained in the far-field as typical Dirichlet boundary conditions. The innermost liquid node serves as the center of origin imposing the no-flux condition. In order to avoid oscillatory solutions, the discretized mass flux is calculated on the cell faces instead of cell centers. The final set of discretized equations are then numerically integrated using a variable higher order backward differencing scheme (up to fifth order) with adaptive time step utilizing implicit multipoint interpolation. All the reported simulation results are obtained using 50 liquid and 150 gas phase nodes. Test results that confirm grid-independency of the solution are separately annexed in the supplementary material as Supplementary Fig. S1.

To investigate the sensitivity of predictions to the chosen ozone kinetics, two different kinetic model sources [24] and [25] were separately appended to the hydrocarbon reduced models. The kinetics appearing in reference [25] are based upon the rate parameters proposed in reference [26]. The predicted behaviors were found to be only weakly dependent on the chosen source of O_3 chemistry. An exemplary illustration of peak gas temperature for a 0.5 mm initial diameter *n*-C_7H_{16} droplet comparing predictions using these two different ozone model sources at two different O_3 seeding conditions is presented in Supplementary Fig. S2. The kinetic model based on the work of Ombrello et al. [25] was used in all of the simulations subsequently reported here.

3. Results and discussion

3.1. Cool flame combustion characteristics of a low flash point temperature fuel – n-heptane

3.1.1. Initiation dynamics and stabilization of cool flame of an n-heptane droplet at 298 K

The potential for direct initiation of cool flame burning for a sub-millimeter size *n*-C_7H_{16} droplet with O_3 addition is first explored conceptually by employing two different initiation energy deposition approaches. In the first, the entire ambient temperature field is raised at time zero from 298 K to 425 K (hot ambient approach). The second approach imposes a predefined trapezoidal shaped high-temperature ambient profile (prescribed thermal

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