Combustion and Flame 194 (2018) 107–114

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

Radiative extinction of large n-alkane droplets in oxygen-inert mixtures in microgravity

Vedha Nayagam[a,*], Daniel L. Dietrich[b], Michael C. Hicks[b], Forman A. Williams[c]

[a] Department of Mechanical and Aerospace Engineering, Case Western Reserve University, Cleveland, OH 44106, USA
[b] NASA Glenn Research Center, Cleveland, OH 44135, USA
[c] Department of Mechanical and Aerospace Engineering, University of California San Diego, La Jolla, CA, 92093, USA

ARTICLE INFO

Article history:
Received 21 February 2018
Revised 24 April 2018
Accepted 24 April 2018

Keywords:
Droplet combustion
Radiative extinction
N-alkanes
Microgravity

ABSTRACT

Experimental observations are presented concerning radiative extinction of large n-alkane droplets in diluent-substituted environments at moderately varied pressures in microgravity onboard the International Space Station. The fuels considered are n-heptane, n-octane, and n-decane with carbon dioxide, helium, and xenon used as inerts, replacing nitrogen as diluents at varying amounts. It is shown that a simple scaling analysis, based on the assumptions that radiative extinction occurs when the flame temperature drops to a critical value and that the radiative heat loss rate is a fraction of the heat-release rate at the flame, is able to correlate the measured droplet diameter at extinction as a function of its initial diameter and of the ambient gas-mixture properties.

1. Introduction

Understanding the conditions under which diffusion flames extinguish is of fundamental interest as well as being of practical interest in industrial applications and in fire-safety evaluations. It is generally understood that diffusion flames can exhibit two different modes of extinction, one caused by insufficient residence time for heat release to occur in the flame, called diffusive or blow-off extinction, and the other dominated by radiative heat loss from the flame, called radiative extinction. These two modes of extinction have been investigated in numerous studies, some of which are worth reviewing here. For the spherically symmetrical droplet-combustion problem, Chao et al. [1] provided an analytical description of diffusive and radiative extinction on the basis of an activation-energy-asymptotic technique. In addition, numerical simulation of the phenomenon with detailed, high-temperature chemistry has been carried out by Marchese et al. [2], among others. Experimental observations of radiative extinction of large n-alkane fuel droplets, burning in air and in oxygen–helium environments, were made in experiments performed the Space Shuttle [3,4].

When either one-step chemistry or detailed chemistry that involves only high-temperature combustion reactions is employed, the results predict that, following radiative extinction, the droplet simply evaporated in the hot environment. Recent space-based droplet-combustion experiments, Flame Extinguishment in Microgravity (FLEX and FLEX-2), conducted onboard the International Space Station, however, revealed that n-alkane droplets, following radiative extinction of the hot flame, experience a transition to a second stage involving quasi-steady combustion controlled by low-temperature cool-flame chemistry [5,6]. The cool flames themselves are observed to extinguish at a finite droplet diameter, depending on the environmental conditions [7]. The extinction diameter of the cool flame was observed to vary with the initial droplet diameter, indicating possible influences of the initial hot-flame combustion history on the second-stage combustion. This result motivated the present attempt to describe radiative extinction of the hot-flame combustion in a simplified manner that can be useful for correlating results of experimental measurements.

The FLEX series of experiments also investigated the flammability of liquid fuels in a variety of inert-substitute environments, where nitrogen in the ambient gas is replaced by other inert gases, such as carbon dioxide, helium, or xenon, in varying amounts, partially to aid in the evaluation of fire-extinguishment strategies in spacecraft. Inert-gas substitution leads to changes in the effective oxygen Lewis number Le_O; lighter weight inerts (e.g., helium) make Le_O greater than unity while heavier inerts (e.g., xenon) make it less. Among the many theoretical analyses of droplet-supported flames with non-unity Lewis number Matalon and Law [8] indicated that, under typical experimental conditions, the effect of the Lewis number can be approximated as a correction to the ambient oxygen concentration by a factor $1/Le_O$, an increase in the

* Corresponding author.
E-mail address: vedha.nayagam-1@nasa.gov (V. Nayagam).

https://doi.org/10.1016/j.combustflame.2018.04.023
0010-2180/

diffusion coefficient of oxygen being as important as an increase in its concentration.

Employing the 2.2-second drop tower at the NASA Glenn Research Center, Shaw and Dee [9] studied small ($\sim$1 mm initial diameter) droplets of mixtures of decane and hexadecane burning in He- and Xe-diluted environments, and they concluded that Soret effects could play a critical role in determining flame temperatures, sooting characteristics, and flame unsteadiness. More recently, Shaw and Vang [10] considered the effects of the oxygen Lewis number on methanol and n-heptane droplet burning in He- and Xe-diluted atmospheres based on results obtained from the FLEX series of experiments. They found that the Limiting Oxygen Index (LOI), the concentration of oxygen below which sustained quasi-steady combustion is not possible, is lower in air/Xe mixtures than in air/He mixtures for both methanol and n-heptane droplets. The analysis of Aharon and Shaw [11] demonstrates the utility of focusing on the oxygen concentration for describing the flame location in droplet burning, as will be done in the present investigation.

More recently, in a computational study, Alam et al. [12] investigated numerically the effectiveness of xenon as a potential fire suppressant considering methanol droplets with initial diameters in the range between 1 and 2 mm. They found that xenon has a significantly lower LOI than argon, carbon dioxide, helium, or nitrogen, qualitatively in agreement with Shaw and Vang [10], and they conclude that when the combination of higher flame temperature, longer burning time, and the lowest LOI are considered together, xenon is not an effective choice as a fire suppressant. More recently, employing detailed chemical kinetics that include both high-temperature and low-temperature combustion paths, Farouk and Dryer [13] performed numerical simulations of two-stage combustion of n-heptane, n-decane, and n-dodecane droplets at normal atmospheric pressure, with a fixed oxygen concentration of 21% by volume in O_2/N_2/He mixtures. Their results showed that, while the hot-flame extinction diameter varied linearly with the initial droplet diameter for n-heptane and n-decane in O_2/N_2 mixtures, a similar trend was not observed in O_2/He mixtures. These computational results supplement the experimental results in underlying the groundwork for the present investigation.

The objective of this study is to develop a unified view of radiative extinction of hot flames using a simplified scaling analysis that captures the observed trends in experimental results from FLEX and FLEX-2 for droplets of n-heptane, n-octane, and n-decane burning in varying diluent-substituted environments at moderate pressures. To the best of our knowledge no such analysis for facilitating treatment of experimental data exist in the current literature.

The rest of the paper is organized as follows: First we present the simplified scaling analysis, followed by a brief description of the experiments, including representative experimental results that illustrate the influences of various parameters on radiative extinction, and finally a dimensionless correlation for the droplet extinction diameters that tests the scaling arguments, using extensive experimental data. A summary of key finding of this paper is provided in the conclusions section.

2. Scaling analysis

2.1. The central energy balance

A simplified model can be developed for describing how radiative extinction comes about during droplet combustion. Following ignition, a hot diffusion flame, with a temperature close to the adiabatic flame temperature T_{ad}, forms at some distance from the fuel surface. The outer surface of the flame then expands with time, resulting in an increased volume of radiating gas, while the heat-release rate decreases slowly because of the shrinking size of the droplet, thereby decreasing the maximum flame temperature. Eventually, the flame temperature reaches a critical value T_{ex} at which the chemical mechanism causes the gas-phase reaction rate to decrease precipitously, resulting in flame extinction. A simple model that captures this essential physics can be expressed as

$$\rho c_P V \frac{dT}{dt} = \dot{Q}_c - \dot{Q}_r, \tag{1}$$

where ρ, c_P, and T are the radiating gas density, specific heat, and temperature, respectively, and t is the time. An effective control volume of the radiating spherical mass is V, $\dot{Q}_c$ is the total chemical heat-release rate within that volume and $\dot{Q}_r$ the total radiative heat loss rate from that volume.

The heat-release rate is approximately $(\pi/4)\rho_\ell q_c d_s K_h$, where ρ_ℓ denotes the liquid fuel density, q_c the heat released per unit mass of fuel burned, d_s the droplet diameter, and K_h the average hot-flame burning-rate constant. This approximation applies when the time difference between liquid-fuel evaporation and gas-phase fuel combustion is sufficiently small, as occurs for the existing small values of ρ/ρ_ℓ. In an optically thin (transparent-gas) approximation, the radiative heat-loss rate from the spherical volume is

$$\dot{Q}_r \approx 4\sigma K_P (T^4 - T_\infty^4) V, \tag{2}$$

where K_P is a Planck-mean absorption coefficient (proportional to the pressure P), the product of the gas density and the mass absorption coefficient, equal to the reciprocal of the Planck-mean absorption length, while σ is the Stefan–Boltzmann constant, and T_∞ denotes the ambient temperature. The approximate equality is employed here and below to denote the correct functional dependence but a need for the introduction of an empirical constant factor, in this case associated with the arbitrariness in the definition of the radiating volume. Typically as the flame expands, the flame temperature drops, and the flame becomes pale blue in color, indicating that the soot-formation process has ceased to occur as the extinction condition is approached. Under those conditions the major radiating species are CO_2 and H_2O, so that the Planck-mean absorption coefficient can be expressed as

$$K_P = P(X_{CO_2} K_{P,CO_2} + X_{H_2O} K_{P,H_2O}), \tag{3}$$

in which the mole fractions X_{CO_2} and X_{H_2O} are to be calculated for stoichiometric combustion of the fuel, with an added contribution from the ambient gas in determining X_{CO_2}, and the associated $K's$, shown here, are pressure-independent.

In terms of the flame radius, r_f, the radiating volume V will be proportional to $(4/3)\pi r_f^3$. After determining r_f, then substituting Eq. (2) and the expression for $\dot{Q}_c$ into Eq. (1) provides an explicit approximate evolution equation for the gas temperature T. A study of the nondimensional form of Eq. (1) showed that the storage term is negligible compared to the heat-release-rate term, and the equation then becomes simply

$$\frac{\pi}{4}\rho_\ell q_c d_s K_h \approx 4\sigma K_P (T^4 - T_\infty^4)\frac{4}{3}\pi r_f^3. \tag{4}$$

This is the basic energy-balance equation that underlies the present scaling analysis.

2.2. The Approximation for the flame radius

The growth of the radiating volume V is estimated by considering the transient evolution of the mixture fraction Z from the time of ignition. Since, when radiative extinction will occur, the flame must migrate to the outer zone where convection is of secondary importance, as a first approximation it is reasonable to neglect the convective effects in writing the solution for the mixture fraction as a function of time and the radial coordinate r. The partial differential equation to be solved for Z then is the diffusion equation in