Effectiveness of Xenon as a Fire Suppressant Under Microgravity Combustion Environment

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ABSTRACT
The ‘Flame EXtinguishment’ (FLEX) program conducted by NASA on board the International Space Station (ISS) has been assisting in developing fire-safety protocols for low gravity applications through microgravity droplet combustion experiments. A wide range of fuels, including alcohols and alkanes, have been studied in different ambient conditions that also encompass the use of various diluent species and concentrations. A prime focus of the work has been to observe the relative effectiveness of atmospheric composition and pressure changes on fire suppression under ‘reduced’ gravity conditions. Here, detailed numerical simulations are performed to investigate the combustion and extinction characteristics of isolated spherically symmetric 1.0–2.0-mm diameter methanol droplets burning in xenon (Xe)-enriched environments. Comparisons of diluent behaviors under identical conditions using argon (Ar), carbon dioxide (CO\textsubscript{2}), and helium (He) as the alternative diluent to nitrogen are also reported. The predictions are compared against ISS experiments with good agreement and with less satisfactory agreement with the results published earlier by Shaw and Wei (2012). Xenon as diluent rather than nitrogen results in reduced burning rate, larger extinction diameter and counter intuitively, and prolonged burning time. The limiting oxygen index (LOI) for xenon is found to decrease significantly from that found with argon, carbon dioxide, or helium. The numerical analyses indicate that the lower thermal diffusivity of xenon is the principal factor responsible for the remarkably lower LOI. Water accumulation within the methanol droplet and its relevance to the extinction process is also discussed. It is concluded that the combined observation of elevated peak gas temperature, its slow decay due to minimal diffusive heat loss, and the exceptionally lower LOI value associated with xenon as a diluent all detract from its utility for suppressing fire concerns in reduced gravity applications.

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Introduction
Combustion of spherically symmetric isolated fuel droplets under quiescent conditions provides well characterized opportunities to obtain fundamental data on the coupling of chemical kinetics and transport in diffusion limited combustion, as well as elementary
combustion properties, such as burning rate, flame structure, extinction phenomena, and limiting oxygen index. Moreover, isolated, spherically symmetric combustion configuration offers opportunities to include substantial detail in the sub-model components describing chemical kinetic, diffusive transport, and radiative interactions. A majority of present fire safety knowledge encompasses situations in which changes in gas density caused from heat generated by the combustion event results in natural convective effects. Evaluating the effects of diluent substitution on fire extinguishment phenomena and the effectiveness of different diluents as fire suppressants under low gravity applications where natural convective effects are absent is important to present as well as future low gravity missions. Observing extinction phenomena under such conditions also provides unique scopes to further understand the role of specific finite-rate chemistry/kinetics, and diffusive/radiative interactions on extinction. Finally, combustion of spherically symmetric liquid fuel droplets is a fundamental advantageous canonical experimental venue to generate data for developing/testing the relevant sub-model components, their simplification, and relative significance toward accurate description of the coupled physical-chemical processes governing liquid fuel utilization (Choi and Dryer, 2001).

For a systematic analysis of different limiting cases, methanol has frequently been a fuel of choice because of its non-sooting combustion behavior; however, the hygroscopic nature of this smallest alcohol introduces other physical complexities (Farouk and Dryer, 2012a). Choi et al. (1988) were first to denote the nonlinear $d^3$-law behavior for methanol droplets burning in air and attributed this behavior to dissolution of combustion products especially water from the gas phase into the liquid droplet. Choi (1992) and Lee and Law (1992) measured the absorbed product during methanol droplet combustion for both free falling and suspended droplets. Their measurements confirmed that a substantial amount of water is absorbed over the droplet combustion lifetime. In a follow-on numerical work, Marchese and Dryer (1996) highlighted the role of liquid phase internal circulation/motion on the water absorption phenomena and showed that the liquid phase within the droplet needed to be assumed as well mixed in order to achieve agreement of predictions and experimental measurements. Dwyer et al. (1996) in their multidimensional numerical work showed that water dissolution in methanol droplets introduces significant surface-tension-driven liquid motions. All of these earlier works suggested that the extinction process of smaller-sized methanol droplets was governed by water dissolution and subsequent gasification effects. Interestingly, compared to methanol, ethanol is less affected by water dissolution due to its azeotropic properties (Kazakov et al., 2003).

Cho et al. (1991) conducted combustion experiments with methanol droplets in He-O$_2$ mixtures to determine extinction diameters. The highly conductive He-O$_2$ environment facilitates higher burning rates that promote extinction in short duration. In an independent study with methanol/dodecanol droplets, it was shown that pure methanol droplets burning in air exhibited extinction at a non-zero droplet diameter (Yang et al., 1991). Chauveau and coworkers (2000) studied methanol droplet combustion at higher pressure and concluded that the $d^3$ law holds true for all ambient pressure up to 1.4 times that of the critical pressure for pure methanol. They also confirmed that the burning rate constant varied as $Gr^{1/4}$. However their experimental burn time never extended to the extinction conditions, where nonlinearity in $d^3$ behavior is prevalent. Further analysis with water absorption and dissolution in methanol droplet combustion revealed that water-dissolution-driven extinction becomes less important at higher pressure (Okai et al., 2000).
Marchese and Dryer (1997) showed that for methanol droplets burning in air, the radiative heat loss becomes increasingly important with initial droplet sizes greater than 1 mm, leading eventually to radiative extinction at sufficiently large diameters. Marchese and Dryer’s work also showed that a wide range of gas-phase Lewis numbers exist for the different species within the flame structure, contrary to assumptions typically applied in asymptotic analyses (Chao et al., 1991; Zhang et al., 1996). In a recent study (Hicks et al., 2010), a number of microgravity drop tower experiments were conducted and analyzed to study the effects of CO$_2$-enriched environments. Although CO$_2$ is a radiatively participating diluent, studies concluded that moderate-sized droplets underwent diffusive extinction with little influence of the changes in radiative transport.

Methanol droplet combustion has been studied numerically in the past (Awasthi et al., 2013; Dwyer and Shaw, 2001; Farouk and Dryer, 2012b; Raghavan et al., 2005, 2006; Zhang et al., 1996). Despite this long standing history, studies pertaining to diluent exchange and effect of diluents on fire suppression behavior from droplet combustion perspective have been relatively few (Farouk and Dryer, 2012a, 2012b, Nakaya et al., 2013; Shaw and Wei, 2011; Wei and Shaw, 2009). The present work substantially advances the study of isolated droplet combustion specifically in xenon-enriched diluent environments over earlier works (Jin and Shaw, 2010; Shaw and Wei, 2012), by considering space-based, larger diameter, experiments and computational models that encompass detailed chemistry, multi-component diffusion, and comprehensive radiative coupling. New simulation results on the effect of xenon on isolated methanol droplet combustion under microgravity conditions are reported based upon a recently developed one-dimensional spherically-symmetric transient combustion model (Farouk and Dryer, 2011, 2012a, 2012b). The model predictions are compared with recent experiments conducted on-board the International Space Station (ISS). Subsequently, numerical predictions of droplet regression, peak gas phase temperature, and flame stand-off ratio (FSR) with varying $\text{O}_2$ (viz. xenon) concentration for different initial diameters are presented. Average burning rate ($K_{o,\text{avg}}$), average FSR, and normalized extinction ($D_{\text{ext}}/D_o$) diameter data as a function of oxygen concentration were evaluated to determine the limiting oxygen index (LOI). The computational analyses also highlight the influence of argon, carbon dioxide and helium on the combustion characteristics (especially LOI) in order to assess diluent effects found with xenon. Finally, analyses are presented concerning methanol droplet water dissolution effects resulting from diluent modifications.

**Mathematical model and numerical schemes**

The transient, spherically-symmetric droplet combustion model utilized here features gas phase kinetics, spectrally resolved radiative heat transfer, and multi-component transport. Details of the model can be found in previous publications discussed above (Farouk and Dryer, 2011, 2012a), and only a brief description of the model is provided here.

For conditions below the critical pressure of the test fuel, the problem is one of two continuum fluid flow domains interfaced by a complex and dynamic boundary separating liquid and vapor states. In this work, local thermodynamic equilibrium and low Mach number conditions are applied. Due to the ramification of the zero-gravity environment for which predictions will be made, the solution of the momentum equation is not
required. The conservation equations for species and energy applicable for the control volume in both phases can be described as:

\[
\int_{r_-}^{r_+} \frac{\partial (\rho_i y_i)}{\partial t} r^2 dr + \frac{r^2}{3} \frac{r^2}{r_- r_+} \int_{r_-}^{r_+} \rho_i (\rho u - \rho \dot{r}) r^2 \bigg|_{r_-}^{r_+} = -y_i \rho V_i r^2 \bigg|_{r_-}^{r_+} + \int_{r_-}^{r_+} \dot{\omega}_i r^2 dr
\]

(1)

\[
\int_{r_-}^{r_+} \frac{\partial (h \rho)}{\partial t} r^2 dr + \frac{r^2}{3} \frac{r^2}{r_- r_+} \int_{r_-}^{r_+} h(pu - \rho \dot{r}) r^2 \bigg|_{r_-}^{r_+} = -q r^2 \bigg|_{r_-}^{r_+} + S_{\text{Loss or gain thru fiber}}
\]

(2)

\[
\sum_{i=1}^{X} y_i = 1
\]

(3)

The heat flux (q) quantity cumulatively represents the contribution from diffusive and radiative heat transfer. The diffusive component is comprised of thermal conduction, enthalpic transport via species diffusion, and Dufour effects where the heat flow is established due to gradients in composition. The diffusive heat flux is expressed as:

\[
q_{\text{diff}} = \sum_{i=1}^{X} h_i \rho_i y_i V_i - \lambda \nabla T_g - p \sum_{i=1}^{X} \theta_i d_i
\]

(4)

Here, \( \theta_i = D_{ij} X_j \)

In addition to the aforementioned features, the model also includes radiative heat transport expressed in the following form. For the sake of convenience, the radiative flux term is only exemplified for a single wave length:

\[
\nabla \cdot \bar{q}_{\text{rad}} = \int_{0}^{\infty} a(\eta, \bar{r}) \left( 4\pi I_\eta (\eta, \bar{r}) - \int_{4\pi} I(\eta, \bar{r}, \omega) d\omega \right) d\eta
\]

(5)

Methanol is hygroscopic by nature, and therefore accurate prediction of the water dissolution/vaporization effects on liquid methanol droplet combustion is critical. The consequence of water absorption has direct impact on quasi-steady burning and flame extinction, and especially for the large droplets associated with the present work, the overall process is also influenced by liquid mass transport within the droplet. For purely diffusive problems, the liquid phase Peclet number is used to characterize the effects of liquid mass transport (Cho et al., 1991; Marchese et al., 1996):

\[
Pe_{l,m} = \frac{r_s |d_\eta|}{D_l} = \frac{1}{8} \frac{d_\eta (d_s^2)}{D_l} = \frac{1}{8} \frac{K_o (t)}{D_l}
\]

(6)

For low Peclet number, the water present at the droplet surface is preferentially diluted throughout the droplet interior, resulting in a reduced diffusive resistance to further water condensation at the droplet surface. On the contrary, a higher Peclet number condition is characterized by a thin layer at the droplet surface containing dissolved water with a slower diffusive migration of water into the droplet interior and hence a reduced rate of
water accumulation within the liquid droplet. As a consequence, negligible water accumulation is observed in the liquid phase over the burning period until very near droplet extinction. In the current simulation, burning rate, $K_o(t)$, is evaluated as part of the solution, with an “effective” liquid diffusivity, $D_l$, provided as an input. As discussed by Farouk et al. (2012a), the “effective” liquid diffusivity, $D_l$, is prescribed by imposing a liquid phase Lewis number, $Le_{liq} = 1.0$, similar to the approach employed previously (Marchese et al., 1996). In the absence of internal liquid motion, the liquid transport is controlled by molecular diffusion and the liquid mass diffusivity of methanol/water system appears to be $\sim 1.5 \times 10^{-3}$ mm$^2$/s (Yeng and Lee, 1991). The higher value of the “effective” liquid diffusivity, $D_l$ (due to the imposed $Le_{liq} = 1.0$), results in the low Peclet number regime (convection or well mixed limit) and corresponds to the enhanced internal fluid motion arising from gas-liquid interfacial effects that include thermal and solutal Marangoni phenomena (Raghavan et al., 2006), interactions induced by droplet formation, growth and deployment methods, and tethering filament surface tension perturbations at the penetration sites on the drop surface. Essentially, it is not possible to produce liquid methanol droplets of nearly any size without initiating and sustaining internal liquid phase motions within the droplet as it burns.

The imposed boundary conditions at the liquid-gas interface arise either through thermodynamic constraints or conservation of material fluxes at the drop surface:

$$y_i(\rho u - \rho \dot{r})|^+_{-} = -y_i\rho V_i|^+_{-}$$

$$\sum_{i_{liquid}} h_{vap,i}y_i(\rho u - \rho \dot{r}) + y_i\rho V_i|^+_{-} = -q|^+_{-} - q_{fiber}$$

$$\sum_{i_{gas}} y_i|^+ = 1$$

$$\sum_{i_{liquid}} y_i|^-_{} = 1$$

$$T|^+_{} = T^-{}$$

$$x_i|^+_{} = x_i|^-_{} = y_i(T, x_j^-)p_{vap,i}(T)$$

The complete set of coupled partial differential and algebraic equations are discretized first in space and then integrated in an automated fashion as a set of coupled ordinary differential-algebraic equations in time. Spatial discretization is performed according to a node-centered finite volume scheme with a second-order accuracy. The gas-liquid interface demarcates the volume boundaries for which the inner zone represents the condensed phase liquid fuel and the outer zone represents the gas phase ambient and the far field (typically two hundred times the initial droplet diameter). The Dirichlet conditions imposed on the far-field are of fixed ambient composition and temperature. The innermost liquid node is centered at the origin, reflecting the no-flux condition. The discretized mass flux is represented on cell interfaces and not cell centers, in the manner traditionally referred to as a staggered grid to avoid oscillatory solutions. Numerical integration of the final set of discretized equations is performed using a backward difference formula with a variable order of up to fifth order and a variable time step utilizing a fully implicit
multipoint interpolation. This method is appropriate for the large range of time scales and stability constraints imposed by a chemically reacting system and automatic time-step variation. All results presented here are obtained using a total of 220 spatial grid points: 70 grids points in the liquid phase and 150 in the gas phase (shown to yield a grid-independent solution).

**Results and discussion**

Numerical simulations of isolated methanol droplet combustion were performed for three different initial diameters, $D_0 = 1.0, 1.5, \text{ and } 2.0 \text{ mm}$ encompassing a broad range of xenon concentrations in the ambient with the $\text{Xe/O}_2$ volumetric ratio systematically varied. Similar computations were also conducted for argon, carbon dioxide and helium diluents. The detailed methanol oxidation mechanism of Li et al. (2007) consisting of 21 species undergoing 93 elementary reactions with the hydrogen oxidation sub-model update of Burke et al. (2012) was employed for this study. The liquid phase properties of methanol were evaluated using the data correlations from Daubert et al. (1989).

The present numerical study was undertaken principally to analyze the recently conducted experiments onboard ISS under the Flame Extinguishment (FLEX) program. The details of the experimental procedures utilized in performing the experiments, including data collection and reduction methodologies, can be found in Dietrich et al. (2014). No additional data processing was performed as part of the current work. From the ISS FLEX test matrix, ‘FLEX 563’ was judiciously chosen for model validation and detailed analysis purposes, since this test used the maximum xenon displacement of nitrogen as diluent ($D_0 = 2.771 \text{ mm, } X_{\text{O}_2} = 8\%, X_{\text{Xe}} = 63\%/\text{balance } \text{N}_2$). Figure 1 compares the predicted droplet diameter regression, flame stand-off ratio, and flame diameter evolution against the ISS experimental data for identical conditions. The simulation results agree well with the measurements ($RMSE_{\text{flame,dia}} = 3.08 \text{ mm (low light level ultra violet camera), } 2.87 \text{ mm (color camera)}; RMSE_{\text{FSR}} = 1.32 (\text{low light level ultra violet camera), } 1.29 (\text{color camera})$). The model captures the nonlinearity observed in the experimental droplet regression data (Figure 1a). The vertical line passing through all three sub-plots indicates the flame extinction location ($t \sim 4.90 \text{ s}$). While the droplet diameter regression predictions are in good agreement, the flame stand-off ratio and flame diameter temporal evolution predictions deviate during the initial stage of burning as well as towards the end of the burn time as droplet extinction is approached; $t > 3.5 \text{ s (Figures 1b and 1c)}$. However, deviations in the flame evolution predictions and experimental data during the quasi-steady burn phase are minimal. The scatter in the experimental data reflects the larger uncertainties associated with the flame diameter determination procedure. These discrepancies arise from the nature of the measurements as well as the methods utilized to extract the flame position. No natural convective effects or significant droplet drift were observed in the selected experiment. Furthermore, the role of natural convection was confirmed to be negligible through analyses that considered maximum flame temperatures between 1000 K and 2000 K and flame diameters based upon maximum temperature location (Choi and Dryer, 2001).

The hot wire approach used to initiate droplet combustion involves several uncharacterized issues—ignition energy, spatial deposition, dynamics, symmetry—that as a result are difficult to prescribe computationally (Dietrich et al., 2014). The total ignition energy
appears to be a key factor influencing droplet combustion behavior, though no accurate experimental characterization is available. Thus, numerical predictions based upon three different levels of total ignition energy, all deposited in similar spherically-symmetric spatial distributions about the initial droplet, were performed to parametrically evaluate its effect. Three ignition-to-combustion energy ratios, ICER (0.01, 0.07, and 0.25) were compared. Ignition energies of these magnitudes are observed to affect only the initial transient burning observations (Figure 1). For an ignition energy lower than 0.4 J, quasi-steady burning could not be established, as also found in an earlier, similar analysis (Farouk et al., 2013). Model predictions were also compared against the data reported by Shaw and Wei (2012), and results are shown in Figure S1 (available online in the Supplemental Material).

The effects of initial droplet diameter and ambient xenon displacement on the predicted temporal profiles of droplet diameter regression, peak gas temperature, and flame stand-off ratio (FSR) are presented in Figure 2. Though a wide range O₂/Xe ambience and

![Figure 1](image-url)
drop diameters were simulated, for visual clarity, Figure 2 only presents the results for three $O_2$ molar fractions (0.21, 0.10, and 0.07) and two initial droplet diameters (1.0 mm and 2.0 mm). The droplet diameter regression rate decreases with an increase in ambient xenon concentration (i.e., decreasing $O_2$) for a given droplet diameter, resulting in a lower burning rate, $K_o$, and a diminished peak gas temperature. Increased xenon displacement reduces the average thermal conductivity and increases specific heat capacity, hence, decreasing thermal diffusivity of the surrounding gas mixture. For the larger diameter case, increasing xenon content results in a decrease in regression rate, an increase in extinction diameter, and a longer burning time. Even at the highest xenon concentration, a quasi-steady burning phase was attainable. In comparison, smaller droplets having identical ambient conditions to the larger diameter cases burned at a faster rate due to lower heat loss and consequentially produced smaller extinction diameters. Unlike results for other diluents (helium, carbon dioxide) at increased loading condition (i.e., low oxygen concentration), higher xenon displacements promote rather than degrade quasi-steady combustion (Farouk and Dryer, 2012a).

The temporal evolution of the peak gas temperature as a function of xenon concentration for the same three exemplar cases is presented in Figures 2c and 2d. An increase in xenon content decreases both the maximum value of the peak gas temperature and the maximum rate of increase of the peak gas temperature ($dT_{\text{max}}/dt$). The lower thermal conductivity and higher heat capacity of xenon are the causes of the changes in early stage temperature evolution. For the same ambient condition, lower peak temperatures occur with increased initial diameter, primarily as a result of radiative heat loss. For instance, at $t \sim 1$ s for 21% $O_2$, 1 mm droplet exhibited a peak temperature of 2212 K while the 2-mm droplet yielded 2020 K, a difference of $\sim 190$ K. As depicted in Figures 2e and 2f, the flame
stand-off ratio (FSR) was found to be weakly dependent on the initial droplet sizes studied and strongly dependent on ambient gas composition. Illustratively, for 21% O₂/79% Xe composition, the FSR during the quasi-steady burn period was found to be ~5.0 for $D_o = 2.0$ mm, which then increased to ~5.5 for $D_o = 1.0$ mm. However, when xenon concentration is raised to 93% from 79% ($D_o = 2.0$ mm), the FSR jumped to ~6.4. In microgravity liquid droplet combustion, the flame locates itself in the region where the fuel and oxidizer are at the stoichiometric condition. Increasing dilution results in a larger radial distance where the stoichiometry condition for fuel-oxidizer mixture occurs, and hence a larger FSR.

The average burning rate ($K_{o,avg}$), average flame stand-off ratio ($FSR_{avg}$), and normalized extinction diameter ($D_{ext}/D_o$) as a function of ambient oxygen content ($X_{O2}$) for initial droplet diameters of 1.0, 1.5, and 2.0 mm are presented in Figure 3. The average quantities were obtained by time-averaging the instantaneous values ($K_o$ and FSR) between $t = 0.1t_b$ and $t = 0.95t_b$, where $t_b$ is the total burn time. We define the total burn time ($t_b$) as the time difference between ignition and extinction and exclude the vaporization phase after extinction. It can be seen in Figure 3a that an increase in the

![Figure 3. Numerical prediction of average burning rate (subplot a), average flame stand-off ratio, $FSR_{avg}$ (subplot b), and normalized extinction diameter ($D_{ext}/D_o$) (subplot c) for different initial methanol droplets under varying O₂/Xe surrounding.](image-url)
ambient xenon content (viz. decrease in oxygen) reduces $K_{o,avg}$. The presence of xenon reduces the thermal diffusivity of the ambient significantly. As a consequence, the energy feedback to the droplet surface from the flame zone diminishes, resulting in lower burning rate. For a small droplet, $K_{o,avg}$ varies almost linearly as a function of ambient xenon concentration. As $D_o$ becomes larger, a nonlinearity is observed at higher xenon content due to an emerging dominance of increasing heat losses at oxygen deprived condition. The nonlinearity at low oxygen concentration indicates radiative heat losses at such conditions (Dietrich et al., 1996).

The variation of the average flame stand-off ratio ($FSR_{avg}$) as a function of ambient oxygen concentration (i.e., increasing xenon concentration) for the same three different initial droplet diameters are depicted in Figure 3b. The $FSR_{avg}$ initially increases with decreasing oxygen content, reaching a peak beyond which it starts to fall drastically. This sharp decline in $FSR_{avg}$ is primarily due to the inability to sustain a quasi-steady burning at reduced oxygen environment, which initiates the flame to relocate itself very close to the droplet surface to compensate the net heat loss of the system. The oxygen content for which the maximum $FSR_{avg}$ occurs defines the LOI, as further decreases in the oxygen concentrations yield to unsustainable (quasi-steady) combustion behavior. Furthermore, at a fixed $O_2$ concentration, larger droplets yield reduced $FSR_{avg}$ values as a consequence of increase in heat loss. Hence, the LOI for different initial droplet diameter is observed to increase as the initial droplet diameter is increased. The LOI for $D_o$ values of 1.0 mm, 1.5 mm, and 2.0 mm were found to be $\sim$4%, 5%, and 6%, respectively. This trend is evident in the normalized extinction diameter results presented in Figure 3c. As the LOI condition is attained, the extinction diameter increases sharply for each of the respective cases. In contrast to the LOI results found for nitrogen [e.g., 11% for $D_o = 1.5$ mm at 1 atm (Farouk and Dryer, 2012a)], the LOI for xenon under similar ambient condition is reduced by a factor of 2.2.

In order to assess the effectiveness of xenon as a diluent candidate to improve fire safety criteria under microgravity conditions, the combustion characteristics of xenon-enriched ambient are compared with those in helium (He), carbon dioxide (CO$_2$), and argon (Ar) augmented atmospheres (Figure 4). The simulations presented in the figure are for $D_o = 1.5$ mm, $X_{O_2} = 21\%$, and balance diluent. Helium is found to produce the maximum burning rate, largest extinction diameter, and shortest burn time. The high thermal diffusivity (see Table 1) of He leads to increased heat transfer to both the droplet surface as well as to the far-field (i.e., a thicker flame structure). The heat feedback to the surface increases the droplet burning rate while the losses to the far-field promotes earlier flame extinction. Droplet combustion for the three remaining diluent cases all show relatively similar lower burning rates and temporal locations for extinction in close proximity to one another. Droplet burning in CO$_2$ has the lowest burning rate $K_o$ (i.e., the slowest droplet diameter regression). The presence of high concentration of CO$_2$ in the ambient (in comparison to nitrogen) reduces the average thermal conductivity, increases the specific heat of the ambient mixture, and increases the heat capacity of the surrounding gas mixture. The overall result is decreased thermal diffusive losses. The radiative heat loss also increases as CO$_2$ is a radiatively participating medium. Droplet burning in CO$_2$ is found to have both the lowest flame temperature and the slowest rate of increase of the peak gas temperature ($\frac{dT_{\max}}{dt}_{\text{max}}$) (Figure 4c). Both the lower thermal conductivity and the higher heat capacity of CO$_2$ contribute to
Figure 4. Computational comparison of diluent effect on methanol droplet combustion: (a) droplet diameter regression, (b) flame stand-off ratio, and (c) peak gas temperature. Subplot (b) Inset figure: average flame stand-off \((FSR_{avg})\) ratio for different diluents. \((D_o = 1.5 \text{ mm, } X_{O_2} = 21\%, \text{ balance diluent, atmospheric pressure.})\)

| Diluent gas | Molecular weight, \(M_{av}\) (kg/kmol) | Thermal conductivity, \(k\) (W/m-K) | Specific heat, \(C_p\) (J/kg-K) | Density, \(\rho\) (Kg/m\(^3\)) | Thermal diffusivity, \(\alpha\) (m\(^2\)/s) |
|-------------|--------------------------------------|-------------------------------------|---------------------------------|--------------------------------|-------------------------------------|
| He          | 4.0026                               | 0.1560                              | 5196.52                         | 0.1604                          | \(1.8712 \times 10^{-04}\)          |
| CO\(_2\)    | 44.0095                               | 0.0168                              | 845.45                          | 1.7730                          | \(1.1108 \times 10^{-05}\)          |
| Ar          | 39.9480                               | 0.0177                              | 634.72                          | 1.6025                          | \(2.1195 \times 10^{-05}\)          |
| Xe          | 131.2930                              | 0.0056                              | 158.31                          | 5.2903                          | \(6.5750 \times 10^{-06}\)          |
| Temperature 300 K |                                |                                      |                                |                                |                                      |
| He          | 4.0026                               | 0.2811                              | 5192.87                         | 0.0688                          | \(7.8711 \times 10^{-04}\)          |
| CO\(_2\)    | 44.0095                               | 0.0493                              | 1126.87                         | 0.7562                          | \(5.7851 \times 10^{-05}\)          |
| Ar          | 39.9480                               | 0.0334                              | 520.50                          | 0.6862                          | \(9.5074 \times 10^{-05}\)          |
| Xe          | 131.2930                              | 0.0116                              | 158.51                          | 2.2562                          | \(3.2559 \times 10^{-05}\)          |
| Temperature 700 K |                                |                                      |                                |                                |                                      |

Properties are evaluated at \(T = 300 \text{ K, 700 K, and 1 atm. Data are from NIST Chemistry WebBook (n.d.).}\)}
the differences observed in the early stages of the temperature evolution with increasing CO$_2$ in the ambient. The decrease in $\frac{dT_{\text{max}}}{dt}$ also results in the shift of temporal location for peak gas temperature towards longer burning times, which is analogous to having a larger flame evolution time from the premixed state at ignition to diffusive controlled combustion. The CO$_2$ presence in the ambient significantly decreases the peak gas temperature within the diffusive flame zone, as well as the rate at which the peak flame temperature decreases over the quasi-steady burn.

The combustion characteristics (burning rate and FSR evolution) in xenon-enriched ambient lies between those found with carbon dioxide and argon. Xenon results in the longest burn time (Figure 4b). From the fire safety viewpoint, it is expected that the more desirable diluent should lead to more rapid extinguishment. Thus, xenon underperforms in achieving this target ($t_{\text{ext,Xe}}/t_{\text{ext,CO2}}/t_{\text{ext,Ar}} \sim$ 4.275 s/4.050 s/3.375 s). Xenon diluent also results in the highest flame temperature (Figure 4c), especially during quasi-steady burning. In fact, xenon exhibits the smallest thermal diffusivity among the studied diluents by several factors (see Table 1). In addition to this transport property, xenon also has a low specific heat, the maximum flame temperature, and reduced diffusive losses, culminating in the lowest LOI compared to other diluents studied (Figure 4b).

Since the $FSR_{\text{avg}}$ has been used as a marker for the LOI, the variation of $FSR_{\text{avg}}$ as a function of ambient oxygen concentration for the different diluents is presented in the inset of Figure 4b. The $FSR_{\text{avg}}$ increases with decreasing oxygen concentration (i.e., increasing diluent concentration) to meet the stoichiometric condition at a further distance from liquid fuel droplet surface. This increase in flame position occurs until the LOI condition is achieved. For the carbon dioxide and helium diluent cases, a limited region of the increasing $FSR_{\text{avg}}$ is observed. For oxygen concentrations lower than the LOI, the $FSR_{\text{avg}}$ falls sharply as the flame development becomes fully transient (no quasi-steady burning is observed). In comparison to argon, the $FSR_{\text{avg}}$ in xenon increases in small increments as a function of oxygen concentration. The slow variation is due to the fact that oxygen has the lowest mass diffusivity in xenon (e.g., at 1000 K, $D_{O2,Xe} = 1.032$ cm$^2$/s < $D_{O2,CO2} = 1.295$ cm$^2$/s < $D_{O2,Ar} = 1.578$ cm$^2$/s < $D_{O2,He} = 6.434$ cm$^2$/s). Consequently, xenon exhibits the lowest LOI, which is directly related to the limiting diffusive transport capabilities. For instance, LOI for $D_0 = 1.5$ mm was found to be 5%, 8%, 21%, and 21% for xenon, argon, helium, and carbon dioxide, respectively. The combination of a very low LOI and long burn times points to xenon being a poor choice as a ‘fire suppressant’ diluent under microgravity conditions.

The influence of the thermal transport properties on the combustion characteristics is further illustrated in Figures 5a–5c. The plots summarize the spatially varying temperature profile for two different conditions, X$_{O2}$ 21%/X$_{diluents}$ 79% ($t \sim 0.0105$ s) and for X$_{O2}$ 10%/X$_{diluents}$ 90% ($t \sim 0.03$ s). The highest peak gas temperature with xenon is clearly discernible. These consistent higher temperature profiles for xenon are a direct consequence of its thermal diffusivity (Figure 5c), which enables xenon ambient to accumulate substantial thermal energy. To the contrary, because of its excessively high thermal conductivity (viz. thermal diffusivity, $\alpha$) helium demonstrates the opposite behavior. The consequence of the unique transport characteristics of xenon is further explored through diluent exchange simulations with nitrogen (N$_2$), reported in Figure S2. These simulations
are performed for $D_o = 1.5 \text{ mm}$ with varying $N_2$/Xe exchange ratio at fixed oxygen concentration ($X_{O2} = 21\%$). Due to exceptionally low thermal diffusivity ($\alpha$), the gas phase temperature is found to monotonically increase with the reductions in burning rate ($K$) and a more prolonged burn time as the volume fraction of xenon is increased.

The methanol chemical kinetic model used in this numerical study does not include the third body collision efficiency for xenon due to the lack of appropriate data in the literature. We assume the third body collision efficiency to be identical to that of argon.

Figure 6 summarizes the sensitivity of the average burning rate at the respective LOI conditions for $D_o = 1.0 \text{ mm}$, 1.5 mm, and 2.0 mm to the xenon collision efficiency factor. Simulations were conducted for efficiency factors relative to argon of 0.5, 1, and 2. The predictions show that the average burning rates of the individual cases are insensitive to the variation in the collision efficiency factor.

Water absorption during methanol droplet combustion is a well-known phenomenon that results from their mutually infinite solubility (Cho et al., 1991). Spatially integrated total water accumulation (at near extinction condition) inside a methanol droplet ($D_o = 1.5 \text{ mm}$) with different diluents is illustrated in Figure 7. The binary diffusion coefficient of

![Figure 5](image_url)

**Figure 5.** Predicted spatial distribution of gas temperature at different time instances for $D_o = 1 \text{ mm}$, $X_{O2} = 21\%$ in different diluents: (a) time, $t \sim 0.0105 \text{ s}$; (b) time, $t \sim 0.03 \text{ s}$. (c) Comparison of thermal diffusivity of different diluents at 300 K and 700 K.
Figure 6. Sensitivity of third body collision efficiency of xenon on the average burning rate for different initial diameters at respective LOI conditions. $D_o = 1.0 \text{ mm } (X_{O_2} = 4\%; X_{Xe} = 96\%); D_o = 1.5 \text{ mm } (X_{O_2} = 5\%; X_{Xe} = 95\%); \text{ and } D_o = 2.0 \text{ mm } (X_{O_2} = 6\%; X_{Xe} = 94\%).$

Figure 7. Predicted overall liquid phase water mass fraction ($Y_{H_2O}$) at near extinction for varying $O_2$ concentration in different diluents. Initial droplet size, $D_o = 1.5 \text{ mm.}$ For helium, only $X_{O_2} = 21\%$ case is shown. Inset figure: binary diffusion coefficient of water in different diluents.

Water in different diluents for a temperature range up to 1000 K is depicted as an inset in the figure. An increase in xenon concentration (viz. decrease in oxygen) results in an increase in overall water mass fraction until the LOI condition is achieved. However, the binary diffusion coefficient of water-in-xenon ($D_{H_2O-Xe}$) (Poling et al., 2000), is lower than...
that for water-in-argon or water-in-carbon dioxide. Thus, it can be inferred that the longer burning time in xenon-enriched ambient enables the methanol droplet to absorb more water during the course of combustion compared to other diluents, despite the lower $D_{\text{H}_2\text{O}-\text{Xe}}$ value. Water accumulation with argon as the diluent is similarly large. Contrary to droplet extinction in carbon dioxide and helium ambient, extinction in xenon and argon can be related mainly to water dissolution that migrates from the flame front location (i.e., combustion generated water; Lee and Law, 1992; Marchese and Dryer, 1996).

Subsequently, the aforementioned droplet cases were simulated again to replicate pure vaporization in various bath gas quiescent ambients for a 5-min time considering 40% relative humidity. Detailed analysis of peak water mass fraction is illustrated in Figure 8. The ambient gas composition strongly influences the amount of water that is absorbed during vaporization of the initially pure methanol droplet. Whereas the methanol is evaporated completely from the remaining droplet in helium, significant fuel fractions were found to remain in the droplets evaporated for the same time period in other diluents, with correspondingly less water absorbed over the evaporation time. These observations are consistent with the binary diffusion coefficients of water-in-diluent trend for the various diluents. The fact that xenon-enriched conditions limit water absorption to the droplet during the pre-ignition stage suggests that extinction diameters measured under such conditions are less likely to be perturbed by droplet growth and deployment procedures in humid atmospheres. For all droplet combustion experiments the droplet formation, deployment till the ignition sources are energized are sufficiently long and can have water dissolution effects from the prior combustion events within the combustion chamber aboard ISS.

![Figure 8. Vaporization study of a methanol droplet under different diluent condition ($D_o = 1.5$ mm, fixed $X_{\text{O}_2} = 21\%$, 1 atm, 40% relative humidity).]
Equally compelling to the above time-dependent discourse, spatial variation of water mass fraction within the droplet, and that in the gas phase is also analyzed. It was stated earlier that the effect of water accumulation inside the droplet can significantly influence the extinction process. Figures 9a–9d summarizes the gas phase water mass fraction distribution against normalized radius \( r/r_{\text{drop}} \) for four different diluents at different time burning times. The initial droplet diameter was set to be 1.5 mm and the simulations were performed at ambient condition \( X_{O_2} = 0.21 \) and \( X_{\text{Diluent}} = 0.79 \). For the case of helium, the \( Y_{H_2O} \) profile remains nearly the same as the droplet approaches extinction. Utilizing the FSR data presented in Figure 4b and correlating those results with the time range investigated here, it is observed that the helium-filled ambient contains water as much as 22.5% (by mass) at the flame location at near extinction condition. Following the same treatment, the maximum estimation of water content near the point of extinction for \( CO_2 \), Ar, and Xe is 11%, 14%, and 6%, respectively. Additionally, the water concentration profile in argon and xenon showed an interesting reversal in trends adjacent to the droplet surface as the droplet approaches extinction—instead of water being absorbed into the droplet, water from the droplet started to diffuse out from the droplet into the gas phase. These interesting observations suggest that not only the water absorption but also its subsequent gasification are important attributes of methanol droplet extinction in argon and xenon bath gases (Nayagam, Figure 9. Predicted spatio-temporal profile of water mole fraction in the gas phase at near extinction and quasi-steady times prior to extinction. Ambient composition: \( X_{O_2} = 0.21 \) and \( X_{\text{Diluent}} = 0.79 \). Identical ignition source and initial droplet, \( D_o = 1.5 \) mm.
The liquid phase spatial distribution of water mass fraction for the above cases is summarized in Figures 10a–10d. Methanol in helium is found to absorb negligible amounts of water during the combustion process with a trace amount being transported at the droplet center. Despite the highest value of $D_{\text{H}_2\text{O-He}}$ among the four diluents, the excessively higher gasification rate ($K_{\text{methanol}}$) in helium literally poses a ‘diffusion barrier’ for water in reaching the droplet surface resulting in negligible amounts of water dissolution. In the carbon-dioxide-enriched ambient, water absorption as high as 40–45% (by mass) can be observed through the extinction process, which is primarily governed by the radiative heat loss effect. Analogous to the gas phase observation, methanol droplet water uptake (at the point of extinction) exceeds approximately 83% and 90% for argon and xenon augmented surrounding, respectively. It is worth mentioning that compared to argon, extinction in xenon-enriched environment takes ~20% additional burn time eventually fostering the observed water absorption in xenon. It has been reported in numerous publications that internal circulation/mixing enhances the water absorption process. In our present simulations a well-mixed droplet is assumed by imposing a liquid phase Lewis number of 1. The influence of the liquid phase Lewis number on the liquid and gas phase water profile was investigated and is reported in Figure S3. It should be noted that a unity Lewis number at the liquid phase resembles a well-mixed condition (i.e., internal circulation), while a value set to ‘zero’ replicates the
absence of internal circulation. Without a well-mixed condition very little water gets absorbed into the droplet and results in much smaller predicted extinction diameters.

**Concluding remarks**

The effectiveness of xenon as a potential fire suppressant for micro-gravity application has been numerically studied using a recently developed transient, spheroid-symmetric droplet combustion model. Methanol was chosen as the model fuel. Three different initial droplet diameters, $D_0$ (1.0 mm, 1.5 mm, and 2.0 mm), were considered. For each of these initial droplet diameters, simulations were performed for varying xenon concentration. A priori predictions against experimental data acquired onboard the ISS were found to agree well with the experimental measurements. Additional numerical computations were performed to further elucidate the role(s) of diluent species and substitution amounts on droplet burning parameters, which are important in terms of fire safety in low gravity environments. The findings of these studies can be summarized as follows:

1. The initial ignition source energy has negligible influence on quasi-steady droplet burning and the associated FSR, with principal influences only on the initial burning transient behaviors.
2. The droplet regression rate decreases with increasing xenon content (i.e., decreasing $O_2$) for a fixed droplet diameter, which eventually contributes to reductions in burning rate and earlier flame extinction at larger diameters.
3. An increase in xenon percentage diminishes both the maximum peak gas temperature and maximum rate of increase of the peak gas temperature ($dT/dt_{max}$).
4. The flame stand-off ratio (FSR) is only weakly dependent on the initial droplet sizes while it is strongly affected by ambient gas composition.
5. The exceptionally low thermal diffusivity of xenon is primarily responsible for the significantly higher peak gas temperature and remarkably low LOI in comparison to helium, carbon dioxide, argon, or nitrogen as diluent.
6. Methanol droplets in the presence of xenon bath gas burn for the longest period of time compared to similar conditions with the other diluents. The unified understanding of longest burn time, maximum peak gas temperature, and lowest LOI conditions clearly suggests that xenon is not an effective choice to improve fire safety characteristics in reduced-gravity environments.
7. The LOI for xenon was found to be $\sim 4\%$, 5%, and 6% for respective droplet sizes of 1.0 mm, 1.5 mm, and 2.0 mm burned at atmospheric pressure conditions. Comparative analysis among four diluents revealed that the LOI was 5%, 8%, 21%, and 21% for xenon, argon, helium, and carbon dioxide, respectively, for the same initial drop diameter ($D_0 = 1.5$ mm).
8. Contrary to the heat loss driven extinction phenomena observed with carbon dioxide and helium as the diluent species, extinction in xenon and argon are found to be primarily influenced by water dissolution and gasification effects.
9. Prior to extinction, gas phase medium may contain significant water content. Helium-filled ambient was found to hold as high as $\sim 22.5\%$ (by mass) of water near the flame zone whereas $CO_2$, Ar, and Xe surrounding accommodated approximately 11%, 14%, and 7% of water, respectively. On the other hand, the liquid
phase maximum water mass fraction for CO$_2$, Ar, and Xe ambient may attain values as high as approximately 8%, 88%, and 93%, respectively.

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**NOMENCLATURE**

- $d_s$: droplet diameter
- $d_i$: thermodynamic driving force, in the form of Stefan–Maxwell equation
- $D_l$: liquid mass diffusivity
- $I$: radiative intensity
- $h$: enthalpy per unit mass
- $h_{vap,i}$: enthalpy of vaporization
- $K_o(t)$: instantaneous gasification/burning rate
- $p$: system pressure
- $p_{vap,i}$: vapor pressure of the $i$th component in its pure state
- $q$: heat flux
- $r$: radius
- $r_s$: droplet radius
- $\dot{r}$: control volume boundary velocity
- $S_{\text{Loss or gain-thru-fiber}}$: Loss or gain due to the tether fiber (if tethered microgravity droplet combustion is simulated)
- $T$: temperature
- $T_g$: gas temperature
- $u$: bulk fluid velocity
- $V_i$: diffusion velocity
- $x_i$: mole fraction
- $y_i$: mass fraction
- $\rho$: mass density
- $\dot{\omega}_i$: rate of species production due to chemical reaction
- $\lambda$: thermal conductivity
- $\theta_i$: thermal diffusion coefficient
- $\chi_i$: thermal diffusion ratio
- $y_i$: activity coefficient
- $\eta$: radiative path length
- $\omega$: solid angle
- $+$: gas phase
- $-$: liquid phase
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