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Water Mist Suppression of Propane-Air Flames: Interpretation of Experimental Results

HARSHA K. CHELLIAH

*University of Virginia
Charlottesville, VA*

BRADLEY A. WILLIAMS
JAMES W. FLEMING

*Navy Technology Center for Safety and Survivability
Chemistry Division*

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14. ABSTRACT We report a modeling study to understand the observed suppression behavior of 14-, 30-, and 42- μ m-diameter water drops on propane-air non-premixed counterflow flames. The model employed is a hybrid Eulerian-Lagrangian formulation for treating the interaction of drops and counterflow non-premixed flames. For treatment of the propane chemical kinetics, a skeletal model was developed with validation against experimental non-premixed counterflow flame extinction conditions and low pressure flame structure data for both propane and methane flames, as well as indirect comparison to experimental methane-air burning velocity results. The degree of drop evaporation and resulting levels of water vapor in the incoming air stream were estimated for the experimental conditions. Comparison of the computational extinction strain rates with the reported experimental measurements shows good agreement in consideration of the degree of mist evaporation in the experimental air stream entering the flame. The current results explain the observed drop dependent suppression behavior in these flames.					
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WATER MIST SUPPRESSION OF PROPANE-AIR FLAMES: INTERPRETATION OF EXPERIMENTAL RESULTS

1. INTRODUCTION

Recent experiments conducted at the Naval Research Laboratory (NRL) [1] have shown that small water drops ($<50\ \mu\text{m}$) are more effective than the banned Halon 1301 in suppressing counterflow, non-premixed propane-air flames. Similar experimental results were also observed for methane-air flames. These findings are consistent with methane-air experiments and modeling studies conducted at the University of Virginia (UVa) [2-4]. While the theoretical model developed to describe the interaction of small water drops with counterflow flames has been validated against experimental data of methane-air counterflow extinction using non-monodisperse drops, its applicability to other hydrocarbon fuel flames had not been tested before. The experimental data set of Zegers et al. [1], which was not modeled in the original study, is a valuable data set for application of the model described in [2-4] for several reasons. Zegers et al. reported the results for several monodisperse mists rather than a single polydisperse drop distribution studied by Lazzarini et al., used a different experimental apparatus minimizing the possibility of apparatus-specific effects causing fortuitous agreement, and used propane fuel. Lazzarini et al. reported results for methane. The purpose of this work is then two-fold: interpretation of previously reported experimental water drop suppression results in non-premixed counterflow propane-air flames and further validation of the multi-phase flame suppression model.

A motivation for constructing a well-validated model is the hope of unraveling fundamental physical-chemical phenomena hidden in experimental data. This approach is particularly useful in complex systems, such as the two-phase reacting flow experiments under investigation here. Such fundamental drop/flame validation models are crucial before proceeding to multi-dimensional complex reacting flow systems. This paper reports a detailed comparison between the model developed at UVa describing the interaction of water-mist with counterflow flames and the NRL experimental propane-air flame extinction data.

2. APPROACH

The details of the hybrid Eulerian-Lagrangian formulation and the solution algorithm developed to predict the interaction between water mist and a laminar counterflow flame are described elsewhere [2]. For a dilute drop loading (i.e. drop separation distance/drop diameter ratio > 20 which holds for mass loading of about 3-4% of $10\ \mu\text{m}$ drops) and under the assumption of negligible drop-drop interaction, the model allows for independent trajectories of water drops from that of the gas, and exchange of heat and mass between the condensed-phase and the gas-phase. Momentum exchange between the drops and the gas is also included in the model via Stokes drag force for small drop Reynolds numbers. The evaporated water vapor can freely interact with the detailed homogeneous chemical reactions and can provide a chemical mechanism for flame suppression. More importantly, the effect of dilution or oxygen displacement by water vapor is also taken into consideration.

In the present work, the above two-phase model was extended to include detailed propane-air kinetics. For treatment of the chemical kinetics, a kinetic model was developed with validation against experimental non-premixed counterflow flame extinction conditions and low-pressure flame structure data for both propane and methane flames, as well as indirect comparison to experimental methane-air burning velocity results [5]. The model is based on a much more comprehensive one proposed by Wang and co-workers [6,7], which has been validated based on global flame propagation/extinction experiments and flame structure measurements for a variety of fuels [6]. The propane mechanism used here for calculation of water mist suppressed flames gives very similar extinction strain rates (within 5 s^{-1}) for propane or methane counterflow flames using dry air as the mechanism of Wang [6,7]. Both mechanisms predict a non-premixed propane-air flame extinction strain rate of $\approx 580 \text{ s}^{-1}$ in excellent agreement with the experimental measurements of Zegers et al. [1].

Details of the extinction strain rate experimental studies are reported in [1]. The burner consisted of two 50-cm long, 1 cm id stainless steel tubes. The burner was enclosed in a 22 cm id, 19 cm long acrylic tube with steel plates on both ends. A ≈ 4 liter/min purge flow of nitrogen was introduced into the bottom plate of the chamber and exhausted out the top. Monodisperse water drops ($\geq \approx 15 \mu\text{m}$ diameter) were generated using a Vibrating Orifice Aerosol Generator (VOAG, TSI Inc. Model 3450) with a mist air-fed dispersion cap to disperse the monodisperse drop stream into an aerosol mist. The mist laden air stream was introduced into the burner from the lower tube. Water drop size, number density, and velocity were determined by a Phase Doppler Particle Anemometer (Dantec Flow Lite Model 58N70/58N80). Fuel was introduced through the top, water-cooled tube. Flames of appropriate flow rate could be stabilized in a 1-cm gap between the two tubes. Experimental local strain rates were determined from velocity measurements on the air side of the flame along the tube centerline using Laser-Doppler Velocimetry by seeding the air with sub-micron diameter alumina particles. Subsequent studies using sub-micron diameter water drops were consistent with the alumina particle-based results.

In the absence of any dispersion or dilution air, the VOAG drop generator produces a stream of drops that are highly monodisperse. Sizing determination studies showed that for the mists studied, all drops in the original stream were characterized by a single $4\text{-}\mu\text{m}$ wide PDPA bin size. In order to distribute the stream into a mist, a dispersion cap and entrainment assembly were employed (Fig. 1b in [1]). Mist dispersion and air entrainment of the highly-monodisperse drop stream into a mist in the burner tube degraded the mono-dispersity slightly. Representative PDPA determined size histograms for the experimental mists taken at 2 mm above the air stream tube exit are shown in Fig. 1. As seen in Table 1, $> 50 \%$ of the water mass for each mist was still contained in three $4\text{-}\mu\text{m}$ wide bins, centered around the title bin. For the $14\text{-}\mu\text{m}$ mist, this value was 90 %.

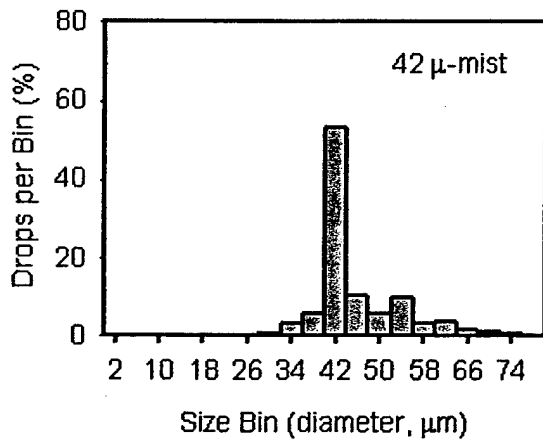
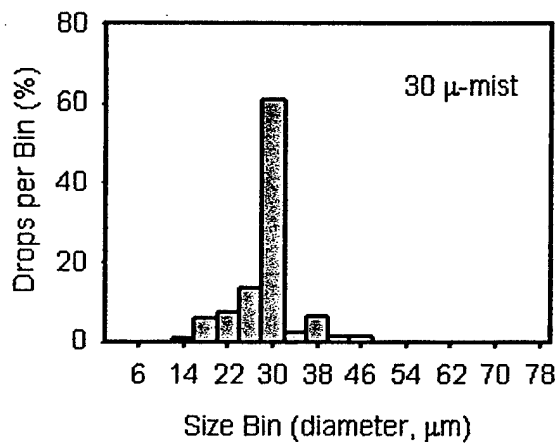
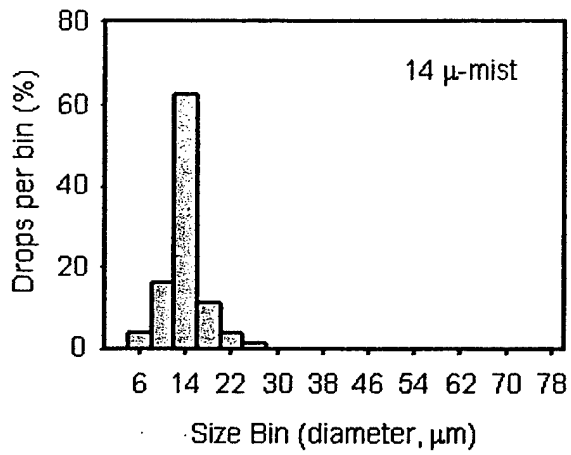


Figure 1 – PDPA determined drop size histogram 2 mm above the air tube exit for the three water mists studied in [1].

Table 1

PDPA derived size information for the mist distribution shown in Fig. 1 measured at 2 mm from the air tube exit.

Mist Name	% water drops $\pm 2 \mu\text{m}$ of nominal size	% water mass $\pm 2 \mu\text{m}$ of nominal size	% water mass $\pm 6 \mu\text{m}$ of nominal size
14 μm	63	47	90
30 μm	61	60	72
42 μm	53	38	51

3. RESULTS AND DISCUSSION

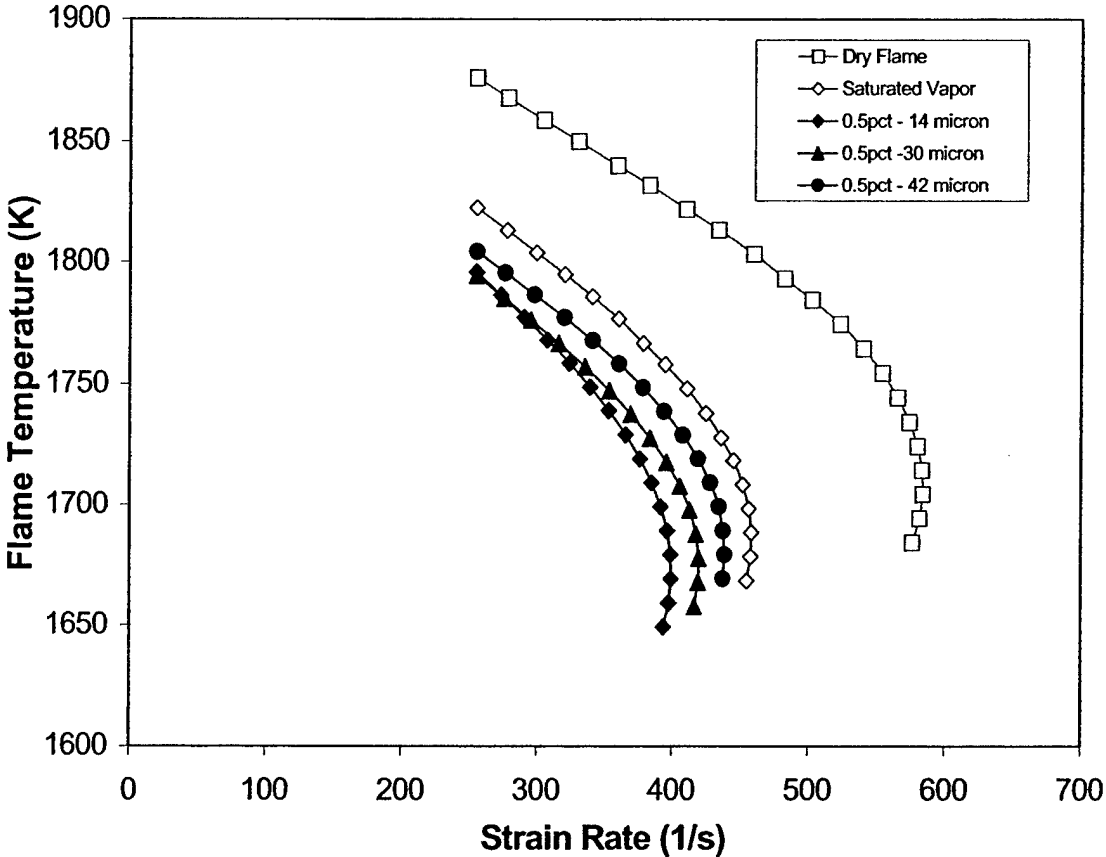
3.1 Effect of Water Vapor

After a sufficient time, an enclosed or semi-enclosed chamber will be saturated with water vapor during the application of water-mist as a fire inhibitor. The time required to attain the saturation condition will depend on several factors, including the air temperature, original humidity level, and the total surface area of the drops applied. For the same condensed water mass, smaller drops have a higher surface area per unit volume (or mass), leading to a more rapid saturation of the initially dry air, while larger drops with lower surface area/volume are expected to take considerably longer. Consequently, different levels of water vapor content in air are realizable (i.e. saturated to partially saturated), depending on the drop size, drop number density or mass added, gas temperature, and the elapsed time.

The model assumes that the room temperature is constant at 300K and the air feed stream is completely saturated with water vapor. The latter implies that drops travel with the air stream long enough to attain equilibrium conditions. At 300 K, the mole fraction of water vapor in saturated air is 0.0352 (3.52%) or by mass 0.0224 (2.24%). This corresponds to oxygen mole fraction of 0.20261, nitrogen of 0.76219 and water of 0.03520 in the inflow stream.

Results of the two-phase model for non-premixed counterflow propane-air flames are shown in Fig. 2. Indicated in the figure are flame temperature versus strain rate curves for flames with dry 300 K air, saturated 300 K air, and saturated 300 K air containing a 14, 30, or

Fig. 2 – Variation of the predicted flame temperature as a function of the flow strain rate for propane-air non-premixed counterflow flames: dry air at 300 K, 300 K air-stream saturated with water vapor, and saturated 300 K air stream with 0.5% mass fraction of monodisperse water drops of diameter 14, 30 and 42 μm



42 μm diameter monodisperse water mist. The extinction condition is defined by the curve turning point; the value of the strain rate at the turning point is the predicted extinction strain rate for each suppressed flame condition. The reduction of oxygen mole fraction from 0.21 (dry air) to 0.2026 (saturated air) due to displacement by water vapor at 300 K yields a decrease in the predicted flame extinction strain rate from 584 to 458 s^{-1} , an almost 22% reduction in the extinction condition, as shown in Fig. 2. At elevated inflow air temperatures assuming complete saturation, the increase in partial pressure of water vapor and the resulting decrease in oxygen concentration in the inflow stream will lead to an even lower flame extinction strain rate. Likewise, a lower level of humidification in the incoming air stream will result in less reduction in the extinction strain rate than that of the completely saturated air condition.

3.2 Effects of Condensed Water and Drop Size

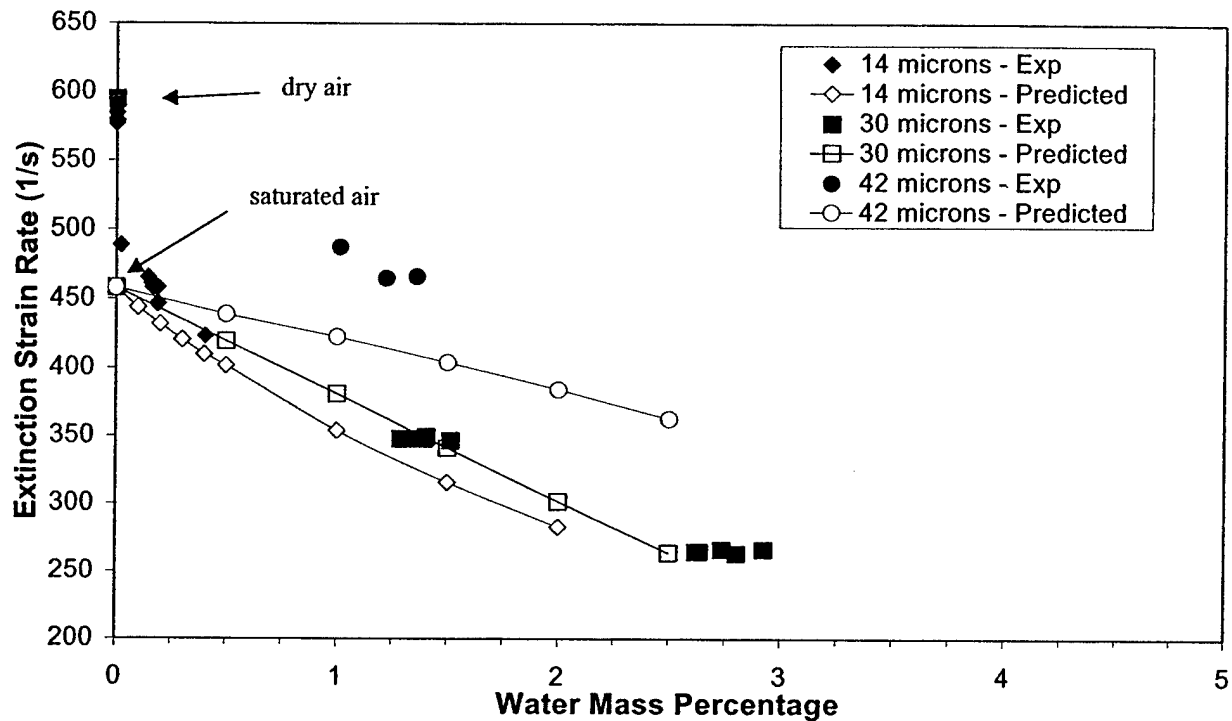
When condensed water drops are added to an already saturated air stream, the interaction of drops with the flame front can reduce the flame extinction condition further, as seen in Fig. 2. However, the degree of reduction of the flame extinction condition will depend on the drop size, consistent with previous modeling and experiments involving the methane-air system [2-4]. Unlike the methane-air counterflow system where the optimal drop size was predicted to be between 15-20 μm [2], the present predictions and experiments indicate that the optimal drop size for the propane-air counterflow system is below 15 μm . The difference in optimal size is related to the higher flame extinction condition of propane-air flames, about 50% greater than that of methane-air counterflow flames. The lower flow residence times at higher strain rates provide less time for a given drop size to completely evaporate. For lower strain rates, drops need to be correspondingly smaller to optimally interact with the flame front.

A comparison of the modeling and experimental results are presented in Fig. 3. Comparison of the effects for the three different mists reveals several phenomena occurring. In the experiments, drops were entrained into dry air. The very rapid reduction in extinction strain rate with only a very small mass of water drops at the flame, followed by a less dramatic fall off with subsequent water drop addition suggests a fair degree of humidification. This is particularly noticeable for the 14- μm mist. The experimental data for the 14- μm mist ≥ 0.005 mass fraction of added water and for the 30- μm data ≥ 0.015 mass fraction of added water drops are in very good agreement with the model predictions. The 42- μm data is $\approx 12\%$ higher than the calculation predicts at 0.015 mass fraction of added water drops. This disagreement is consistent with the degree of humidification for this larger drop size. A quantitative prediction of the degree of air saturation expected for the experimental conditions follows below.

3.3 Humidification Effects of Air Stream

In order to quantify the degree of drop evaporation for the different drop sizes and the effect on flame extinction, evaporation times for the 14, 30, and 42 μm diameter drops were calculated. The calculation incorporates the drop evaporation equations given in [8]. Drop evaporation times in air at 296 K were determined for a range of relative humidity for each of the

Fig. 3 – Flame extinction condition of water mist suppressed propane-air non-premixed counterflow flames showing the local extinction strain rate versus mass fraction of condensed-phase water in the air stream: experimental results from [1] (filled symbols), and calculated results for 14, 30 and 42 μm diameter monodisperse water mists dispersed in saturated air at 300 K (open symbols)



experimental drop sizes. For each drop size, the variation in drop evaporation times between 0 and 100% relative humidity was fit to a second order polynomial.

Next, the evaporation over time of an ensemble of monodisperse drops at a specified initial mass fraction in dry air was determined by a direct time integration. For each 1 millisecond time step, the amount of vaporization was calculated based on the instantaneous relative humidity, the drop number density, and the D-squared evaporation law. The amount of water vaporized impacts the relative humidity and consequently the evaporation rate for the next time step.

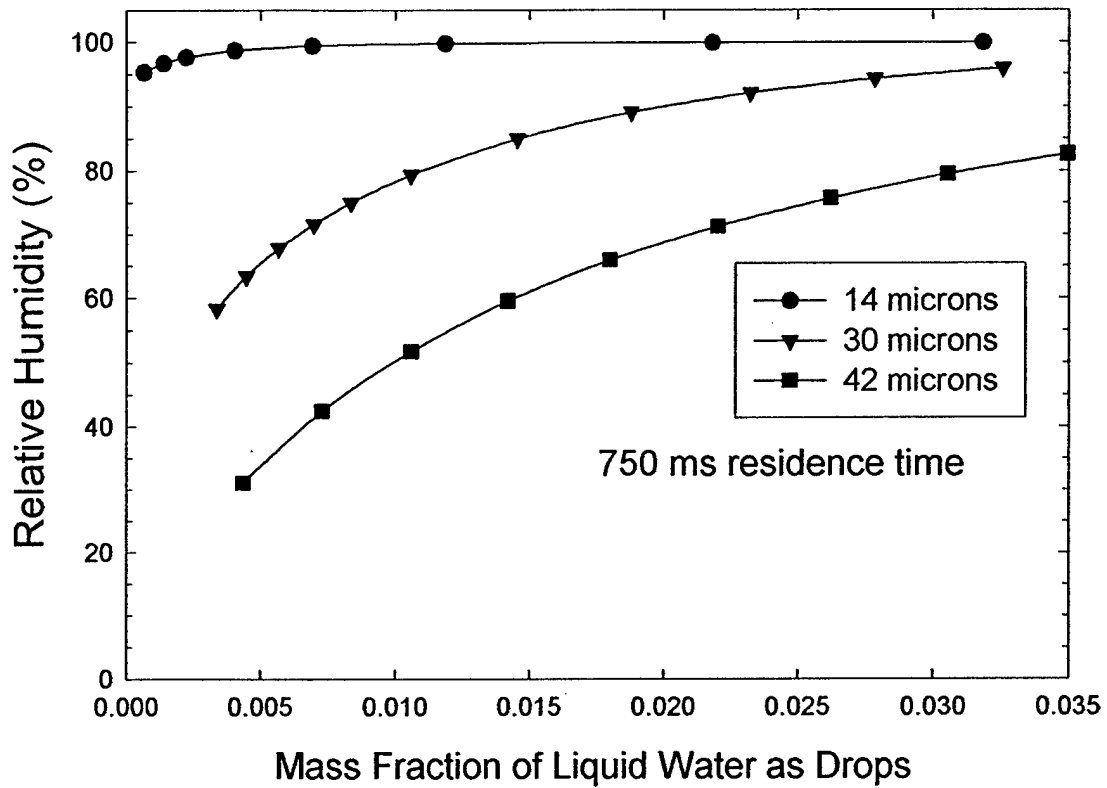
The predictions of the total amount of evaporation for a residence time of 750 milliseconds are shown in Fig. 4. The residence time considered here is the time required to transport the mist after entrainment in originally dry air up the 50-cm long inlet tube. A residence time of 750 ms is the shortest value in the study of Zegers et al. [1], and corresponds to the air exit velocity necessary to produce flames with a local strain rate of $\approx 600 \text{ s}^{-1}$. The shortest residence time provides a lower bound for the degree of humidification. Figure 4 plots the relative humidity (saturated air having a water mass fraction of 0.018 at the experimental temperature of 296 K) against the mass fraction of liquid water remaining after the specified residence time. The liquid water delivered to the flame as determined via PDPA measurements 2 mm above the air tube exit was reported by Zegers et al., rather than the initial mass fraction of water introduced by the drop generator.

Figure 4 shows that in the case of 14 μm drops, for any liquid water to remain after 750 milliseconds, the air stream relative humidity must be at least 95%. Thus the assumption of saturated air in the extinction calculation is valid and is consistent with the rapid reduction in extinction strain rate observed for this drop size. For the 30 μm drops, two sets of experimental points were collected, clustered at liquid mass fractions of 0.015 and 0.028. For the 0.015 mass fraction, the relative humidity after a 750 ms residence time is predicted to be approximately 85%, while for the 0.028 mass fraction it is 95%. Since the extinction strain rates for the flames inhibited by the 30 μm drops in [1] were approximately 350 s^{-1} , this implies a drop residence time in the air stream prior to arrival at the flame of approximately 1250 ms. The degree of saturation for an 0.015 mass fraction of residual liquid at 1250 ms is predicted to be 96% (data not shown). For the 42 μm drops the experimental measurements all had liquid mass fractions in the vicinity of 0.012. For this condition, the calculation predicts a relative humidity of only 55%; assumption of a residence time of 1000 ms, based on the measured extinction strain rate, gives a relative humidity of 66%. The calculation assuming 100% relative humidity would be expected to over predict the extinction strain reduction (lower extinction strain rate), due to the additional heat capacity from the water vapor that was not present in the experiment. This underestimate in the extinction strain rate is in quantitative agreement with the results for the 42 μm mist as shown in Fig. 3.

4. CONCLUSIONS

This paper reports the results of a modeling study to interpret the observed effect of water-mist drop size (in the range of 14 – 42 μm) in suppressing propane-air counterflow flames.

Fig. 4 – Calculated humidification levels of a 296 K air stream containing 14, 30, or 42 μm drops, following a residence time of 750 ms starting in dry air, as a function of the mass fraction of liquid water remaining after drop evaporation.



The agreement between the predictions and experiments are remarkable, considering the high effectiveness of the small amount of water mass introduced to the flame with the air stream. Computations utilized a chemical kinetic propane combustion mechanism that well predicts the measured local propane-air extinction strain rate and a hybrid Eulerian-Lagrangian multi-phase flame suppression model. Water drop suppression modeling of the flames and consideration of the amount of humidification of the air stream for the reported experimental mists quantitatively account for the observed response of the flames to the added liquid water mass as well as the effect of water drops in this size range.

5. ACKNOWLEDGEMENTS

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