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 O S T I

A SPRAY-SUPPRESSION MODEL FOR TURBULENT COMBUSTION

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ABSTRACT

A spray-suppression model that captures the effects of liquid suppressant on a turbulent combustive flow is developed and applied to a turbulent diffusion flame with water spray suppression. The spray submodel is based on a stochastic separated flow approach that accounts for the transport and evaporation of liquid droplets. Flame extinguishment is accounted for by using a perfectly stirred reactor (PSR) submodel of turbulent combustion. PSR pre-calculations of flame extinction times are determined using CHEMKIN and are compared to local turbulent time scales of the flow to determine if local flame extinguishment has occurred.

The PSR flame extinguishment and spray submodels are incorporated into Sandia's flow fire simulation code, VULCAN, and cases are run for the water spray suppression studies of McCaffrey for turbulent hydrogen-air jet diffusion flames. Predictions of flame temperature decrease and suppression efficiency are compared to experimental data as a function of water mass loading using three assumed values of drop sizes. The results show that the suppression efficiency is highly dependent the initial droplet size for a given mass loading. A predicted optimal suppression efficiency was observed for the smallest class of droplets (*i.e.* $D_d = 5\mu\text{m}$) while the larger drops (*i.e.* $D_d = 25$ and $50\mu\text{m}$) show increasing suppression efficiency with increasing mass loading for the range of mass loadings considered. Qualitative agreement to the experiment of suppression efficiency is

encouraging, however quantitative agreement is limited due to the uncertainties in the boundary conditions of the experimental data for the water spray.

NOMENCLATURE

- C_P, C_d Specific heat.
- D_d Droplet diameter.
- F_{D_j} Droplet force due to drag.
- F_{b_j} Droplet force due to body forces.
- h_{lg} Heat of vaporization.
- k Turbulent kinetic energy.
- \dot{m}_d Droplet mass loss term.
- m_d Droplet mass.
- N_d Number of droplets.
- P Pressure.
- \dot{Q}_{dc} Droplet heat source/sink due to convection.
- \dot{Q}_{de} Droplet heat sink due to evaporation.
- S_d Gas phase source terms due to droplets.
- R Gas constant.
- t Time.
- t_{flow} Local representative turbulence time scale.
- $t_{chemical}$ Local representative chemical time scale.
- $t_{blowout}$ Blowout time for a perfectly stirred reactor calculation.
- T Temperature.
- Y Mass fraction of water vapor.
- u_{d_j} Droplet velocity.
- u_{g_j} Gas velocity.

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V_c Volume of computational cell.
 $X_{LIM_{mixture}}$ Suppressant mole fraction.
 $X_{relative}$ Suppressant mole fraction divide by total suppressant mole fraction.

Greek

α Temperature weighting parameter.
 ϵ Dissipation of turbulent kinetic energy.
 ν Kinematic viscosity.
 ρ Density.

Nondimensional Parameters

B_m Mass transfer or Spalding number.
 B_t Thermal transfer number.
 Bi Biot number.
 C_D Coefficient of drag.
 Da Damköhler number.
 Pr Prandtl number.
 Re Reynolds number.
 Sc Schmidt number.
 Sh Sherwood number.
 Nu Nusselt number.

Subscripts

c Thermodynamic critical condition.
d Droplet conditions or properties.
f Film conditions.
g Gas conditions.
ref Reference film saturation conditions.

Superscripts

* Gas phase source terms for a nonevaporating spray.
** Gas phase source terms for an evaporating spray.

INTRODUCTION

The purpose of this research is to develop a numerical simulation capability for the use of liquid sprays in fire suppression with physics based models. The use of this capability is to assess the performance of Halon alternatives driven by the ban of Halon specified by the Montreal Protocol. One alternative for Halon that has received a great deal of attention is the use of fine water sprays. The main physical mechanisms for flame suppression using water sprays include the effects of thermal cooling due to evaporation and gas phase heat capacity, oxygen displacement and radiation attenuation due to the liquid spray.

A partial summary of the research in the use of water sprays as a suppressant can be found in the reviews by Tatem *et al.* (Tatem *et al.*, 1994), Jones *et al.* (Jones and Nolan, 1995) and Mawhinney (Mawhinney and Richardson, 1996). More recent numerical studies in this area can be found in the works of Chow *et al.* (Chow and Fong, 1993), Novozhilov *et al.* (Novozhilov *et al.*, 1996) and Prasad *et al.* (Prasad *et al.*, 1998b; Prasad *et al.*, 1998a; Prasad *et al.*, 1999). Numerical suppression studies of Prasad *et al.* focused on the optimization

of water sprays for the suppression of low Reynolds number (*i.e.* laminar) jet diffusion flames (Prasad *et al.*, 1998a; Prasad *et al.*, 1998b) and pool fires (Prasad *et al.*, 1999). The results of these studies demonstrate that suppression efficiency is highly dependent on the size of the water spray droplets as well as the location of the injection. Optimal suppression was observed when small drops are injected up through the base of the flame. These conclusions are also supported in the work of Novozhilov *et al.* (Novozhilov *et al.*, 1996) and Chow *et al.* (Chow and Fong, 1993) for enclosure fires.

Novozhilov *et al.* show reasonable agreement to experimental data by only considering the thermal effects of the spray indicating that the chemical effects of water vapor on exothermic reaction kinetics are not significant. Lentati *et al.* (Lentati and Chelliah, 1998) supports this idea in their study with examining the thermal and chemical suppression effects of water spray in a counter flow diffusion flame. Their results also indicate that the chemical suppression effects of water vapor contributes little (less than 10%) to the overall temperature drop indicating that thermal cooling due to evaporation of the water spray accounts for the majority of the suppression.

The complete understanding of spray suppression of a turbulent fire involves knowing the intimate coupling of liquid evaporation, turbulence, finite rate chemical kinetics and radiation heat transfer. The objective of this work is to try to account for the first three of these physical processes through subgrid modeling for application to turbulent reacting flows of engineering interest.

The rest of this paper first starts with a detailed descriptions of the subgrid models to account for thermal cooling (spray submodel) and chemical kinetics effects (PSR submodel) in the Mathematical Model Formulation. Results are then presented with comparison to the H_2 - air jet diffusion flames of McCaffrey (McCaffrey, 1984). The comparisons are presented in terms of a decrease in flame temperature as a function of water spray mass loading and droplet sizes. Lastly, conclusions are drawn as to the findings of this study and suggestions for future work.

MATHEMATICAL MODEL FORMULATION

In the interest of brevity, the following mathematical development only summarizes the spray and flame extinguishment model formulations to account for the thermal and chemical effects of a liquid suppressant, respectively. The models are implemented into a general purpose fire simulation code, VULCAN, which is based on the KAMELEON-Fire code (Holen *et al.*, 1990). VULCAN uses a RANS based model suite including a $k - \epsilon$ turbulence model (Jones and Launder, 1972), the EDC combustion model (Byggstøl and Magnussen, 1978), a soot model

(Magnussen, 1981), and a radiation model (Lockwood and Shah, 1981). The gas phase conservation equations are discretized on a staggered, block-structured grid with second-order upwind differencing for the convective terms using a version of the SIMPLE algorithm (Patankar, 1980). Previous studies using VULCAN for pool fire simulations can be found in references (Gritz et al., 1995; Tieszen et al., 1996; Gritz and Nicolette, 1997).

Spray Submodel

The suppression model is based on a stochastic separated flow approach (Faeth, 1987). Transport equations for mass, momentum and energy are integrated in time for groups of droplets (parcels).

$$\begin{aligned}\frac{dm_d}{dt} &= \dot{m}_d = 2\pi D_d \rho_f \frac{\nu_f}{Sc_f} \log(1 + B_m) Sh_f \\ m_d \frac{du_{di}}{dt} &= F_{D_j} + F_{b_j} \\ &= \frac{1}{8} \rho_g D_d^2 C_D |u_{g_j} - u_{d_j}| (u_{g_j} - u_{d_j}) + g \delta_{1i} \quad (1) \\ m_d C_d \frac{dT_d}{dt} &= \dot{Q}_{dc} + \dot{Q}_{de} \\ &= 2\pi D_d \rho_f \frac{\nu_f C_{Pf}}{Pr_f} (T_g - T_d) \frac{\log(1 + B_t)}{B_t} Nu_f \\ &\quad - \dot{m}_d h_{lg}\end{aligned}$$

In Eq.(1) the Sherwood (Sh_f) and Nusselt (Nu_f) transfer numbers are expressed in terms of film conditions using the simple correlations, $Sh_f(or Nu_f) = 1 + Re_d^{1/2} Sc_f(or Pr_f)^{1/3} / 3$, and the coefficient of drag (C_D) is modeled using that for a sphere, $C_D = 24(1 + Re_d^{2/3}) / 6$ for $Re_d (= \rho_g D_d / \nu_f) < 1000$ and $C_D = 0.44$ for $Re_d > 1000$ (Shuen et al., 1983).

The thermodynamic properties at the droplet film surface are obtained by using a thin-skin approximation (Faeth, 1987) where the film temperature is approximated as a weighted average of the droplet and surrounding gas temperatures, $T_f = \alpha T_g + (1 - \alpha) T_d$. In this study, $\alpha = MIN(C_{Bi} Bi, 1)$ where $Bi (= hD/k_f)$ is the thermal Biot number. The model constant C_{Bi} defines the transition Bi number for which the droplet can be treated using a lumped capacitance approach (i.e. $T_d \simeq T_f$) and is set equal to 0.5. The motivation for this model is to account for rapid changes in droplet temperature as it is transported into a flame zone. The use of a simple 1/3 rule (Crowe et al., 1998) resulted in non-physical values of temperature and species mass fractions. The film is assumed to be at saturation conditions so that a partial pressure can be calculated using a Clausius-Clapeyron relation,

$P_f = P_{ref} \exp[-h_{lg}/R(1/T_f - 1/T_{ref})]$ where heat of vaporization, h_{lg} , is allowed to change as a function of temperature using Watson's relation (Watson, 1931; Lefebvre, 1983) (i.e. $h_{lg} = h_{lg_{ref}} [(T_c - T_f)/(T_c - T_{ref})]^{0.38}$). Once the partial pressure is determined then the mass fraction of water vapor is calculated from the ideal equation of state, $Y_f = MW_{H_2O}/MW_g(P_g/P_f - 1 + MW_{H_2O}/MW_g)$. Lastly, the mass (B_m) and thermal (B_t) transfer numbers needed in Eq.(1) are obtained from their definitions as derived from steady-state droplet analysis: $B_m = (Y_g - Y_f)/(Y_f - 1)$ and $B_t = C_{Pf}(T_g - T_f)/h_{lg}$ (Sirignano, 1999).

Droplet dispersion due to turbulence is implemented using both parcel and subparcel models. The parcel model accounts for the effects of large scale turbulent eddies perturbing a parcel trajectory and is based on the random walk model of Gosman and Ioannides (Gosman and Ioannides, 1981) as modified by Shuen et al. (Shuen et al., 1983). Turbulent dispersion of the droplets within a parcel are accounted for using the group modeling concept of Zhou and Yao (Zhou and Yao, 1992) where the spatial distribution of droplets within each parcel are assumed to have a Gaussian distribution.

Flame Extinguishment Submodel

To account for the first order effects of the water spray on the exothermic chemical reactions in a flame, a sub-grid modeled was developed based on PSR theory as formulated by Glarborg et al. (Glarborg et al., 1986) in the CHEMKIN II (Kee et al., 1990) software package. The model is constructed through a sequence of PSR precalculations that map out chemical extinction time scales as a function of temperature and suppressant mixtures. For the current study, the suppressants include H_2O , N_2 , and combinations. In general, extinction times are functions of suppressant mixtures, temperature and pressures and could be used in a tabulated lookup form. However, in order to reduce the storage requirements of such a table, mixing rules are used instead that allow for the mixture mole fraction of suppressant to be determined using the expression (Saito et al., 1999),

$$\frac{1}{X_{LIM_{mixture}}} = \sum_{species} \left(\frac{X_{relative}}{X_{LIM_{species}}} \right) \quad (2)$$

where $X_{LIM_{mixture}}$ is the suppressant mole fraction that extinguishes the flame for a specific suppressant species, $X_{relative}$ is the mole fraction of that particular suppressant species divided by the total suppressant mole fraction, and $X_{LIM_{mixture}}$ is the suppressant mole fraction for extinction for the suppressant in the specific fuel/air mixtures. These mixing rules only work for suppressants that are mostly

thermal in nature (Saito *et al.*, 1999) and so are well suited for studying the effects of water on flame suppression. An example of a chemical extinction time scale calculation is illustrated in Figs. 1 (a) and (b). These figures show the amount of N_2 and H_2O required for extinguishment of an H_2 - air mixture as a function of residence time and temperature from the PSR-CHEMKIN calculations and using the curve fits. Mixtures of H_2O and N_2 are handled using the results of Figs. 1 and the mixing rules of Eq. (2). The results show that, consistent with physical intuition, less suppressant is required to extinguish a flame with decreasing residence times ($t_{PSR_{blowout}}$) and more suppressant is required for extinguishment at higher temperatures. The VULCAN fire simulation package makes use of the PSR precalculations by assuming that the effective chemical time scale at the subgrid can be represented by a PSR so that $t_{chemical} = t_{PSR_{blowout}}$ and compares this time scale to a representative turbulence time scale at the subgrid, t_{flow} , which is estimated from classical turbulence theory, i.e. $t_{flow} = \sqrt{(\nu/\epsilon)}$. If $t_{flow} < Da_{crit} t_{PSR_{blowout}}$, then blowout is assumed to occur and the reactions rates in the EDC combustion model are set equal to zero. The calibration parameter, Da_{crit} , for the model is the critical Damköhler number for extinguishment and is calibrated from jet blowoff studies to a value of 1.367 (Tieszen and Lopez, 1999). A similar criteria for flame extinguishment has been recently used by Koutmos for LES, but Da_{crit} comes from a dynamic length scale ratio rather than assumed constant (Koutmos, 1999). More details on the PSR flame extinction model formulation and its calibration can be found in reference (Tieszen and Lopez, 1999).

NUMERICAL IMPLEMENTATION

The droplet transport equations of Eq. (1) are numerically integrated using the LSODE package for solving systems of stiff ODEs (Radhakrishnan and Hindmarsh, 1993). Gas phase properties needed for the evaluation of droplet transport processes are determined using linear interpolation from the Eulerian grid of the CFD calculations. The effects of the spray are coupled to the gas phase equations through appropriate source terms in the gas phase transport equations and are summarized in Table 1. The source terms are integrated into the gas phase transport equations using a dynamic time-splitting subcycling procedure similar to Amsden (Amsden *et al.*, 1985) to allow for a numerically stable solution of problems involving rapidly evaporating sprays.

The VULCAN simulations presented here employ a $77 \times 26 \times 26$ grid to discretize a $0.1m \times 0.1m \times 0.5m$ domain and are shown in Fig. 2. The simulations are first run 6666 time steps to simulate 0.1 msec of physical time to yield a steady-state solution of the lifted turbulent diffusion flame

as shown in Fig. 3. At 0.1 msec the spray is injected and the gas phase solution integrated another 3333 time steps (0.05 msec) to allow for transients to advect out of the domain and the another 6666 time steps (0.1 msec) for gathering of ensemble statistics. During the transient period 5000 parcels are injected into the flow. Another 10000 parcels are injected for the collection of statistics that involve 1000 realizations of the flow field to construct ensemble mean and RMS statistics.

RESULTS

In this study, the H_2 - air jet flame suppression results of McCaffrey (McCaffrey, 1984) are used for comparison to VULCAN predictions using the new spray-suppression model. This experiment was chosen because of the low levels of luminous radiation from soot. Also, to the authors knowledge, the studies from McCaffrey (McCaffrey, 1984; McCaffrey, 1989) are some of the few experimental studies in the literature that deal with the suppression of simple, easily modeled, turbulent flames. The specific case chosen from the H_2 - air experiment is the 13.7 kW flame (flame B of McCaffrey) for which the hydrogen mass flow rate is equal to 0.11 g/sec producing a jet inlet velocity of 715 m/sec. In the experiment the water spray was injected through the base of the flame using a pneumatic atomizing nozzles which allow for the creation of very small drops. The exact size distribution of the droplets from the experiment was not reported and estimates from the manufacture of the atomizer could not be obtained. Instead three different drop sizes of $D_d = 5, 25$ and $50\mu m$ are used to investigate the effects of drop size on flame suppression. These drop size classes are used for three different mass loading of $\dot{m}_{H_2O}/\dot{m}_{H_2} = 3.66, 5$ and 10 that span the range of conditions from the experiment.

Figure 3 shows centerline cross-sectional contours of flame temperature from the VULCAN simulation at steady-state without the influence of spray. The flame is lifted to a height of around 0.1 m and achieves a peak flame temperature of around 2427K. Comparisons of mean centerline temperature to the experiment in Fig. 5 show relatively good agreement of the flame lift off height location but with a max 15% over prediction error in temperature near the base of the flame. These errors can be attributed to the use of the simple one-step combustion EDC model and the flame extinguishment submodel which does not decrement the combustion rate for reactions close to extinction, i.e. extinction is modeled as an all or nothing event.

Figures 4 (a) and (b) show predictions of instantaneous flame temperature contours and location of the spray parcels for a mass loading of $\dot{m}_{H_2O}/\dot{m}_{H_2} = 5$ using the smallest, $5\mu m$, and the largest, $50\mu m$, drops considered. The plots show qualitatively the sensitivity of flame sup-

pression to drop size. In the first case using the smaller drops, the spray quickly evaporates within the flame causing a dramatic drop in the gas phase temperature to a peak value of 1729K. For the larger drops of Fig. 4 (b), the drops follow a more ballistic trajectory passing quickly through the flame zone before evaporation can take place. This case produces a more modest drop in temperature to a peak of 2442K. These observations are consistent with that of Prasad *et al.* for laminar coflow diffusion flames (Prasad *et al.*, 1998a).

Figure 5 shows a comparison of predicted and measured temperature along the centerline of the jet using the three classes of drop sizes for a mass loading of $\dot{m}_{H_2O}/\dot{m}_{H_2} = 3.66$. The prediction trends suggest that smaller $5\mu m$ droplets are able to pick up the initial drop in temperature at the flame base at around $Z = 0.12m$ but the larger $50\mu m$ drops agree better with the experimental data further downstream (*i.e.* $Z > 0.18m$).

One of the engineering quantities of interest for suppression studies is suppression efficiency. McCaffrey (McCaffrey, 1984) defines spray efficiency in terms of a decrease in flame temperature from the non-suppressed flame, ΔT , divided by the spray mass loading, $\dot{m}_{H_2O}/\dot{m}_{H_2}$. Figure 6 shows spray efficiency comparisons versus mass loading and drop size at the centerline for $Z = 0.122m$. The predictions indicate, that for the smallest drop sizes, an optimal suppression efficiency exists. Physically, this optimum exists because at low mass loadings all of the small drops evaporate in the flame zone so that an increase in water concentration leads to a very large decrease in temperature. However, as the water mass loading is increased, not all of the spray can evaporate in the flame zone and some of it passes through the flame to evaporate further downstream. This case results in a "saturated" suppressed flame state where further increase in mass loading will only lead to a modest decrease in flame temperature. This trend can further be seen in Fig. 7 showing average droplet diameter along the jet centerline versus downstream distance for all cases. For the small droplet $5\mu m$ cases, the average droplet diameter is highly dependent on the mass loading and the penetration distance. Optimum spray loading occurs when all the spray evaporates just beyond the flame zone, *i.e.* for $\dot{m}_{H_2O}/\dot{m}_{H_2} = 5$. The average droplet diameter for the 25 and $50\mu m$ cases are not as sensitive to mass loading as the smaller drops because most of the spray for these cases already passes through the flame zone.

For the 25 and $50\mu m$ drop cases, a different predicted trend is observed. A continual increase in suppression efficiency with increasing mass loading. A partial reason for this trend is the difference in evaporative residence times for the low and high mass loading cases that can be explained in terms of mean droplet and gas phase veloci-

ties shown in Fig. 8. For low and medium mass loading cases (*i.e.* $\dot{m}_{H_2O}/\dot{m}_{H_2} = 3.66$ and 5) the gas phase velocity shows a dramatic drop in velocity to 40m/sec as the flow approaches the lifted flame followed by an acceleration through the flame to 55m/sec due to thermal expansion. For these cases, the drops follow a similar but lagged history slowing down to 33m/sec and then accelerating to around 50m/sec therefore allowing only a short time for evaporation to take place. However, for the high mass loading case ($\dot{m}_{H_2O}/\dot{m}_{H_2} = 10$) we see that the gas and droplet velocities are lower and do not experience much acceleration due to thermal expansion therefore resulting in longer evaporation times in the flame zone. This lower velocity is due to a reduction in thermal expansion due to overall lower temperatures in the flame as well as the increased effects of droplet drag on the gas phase with the larger mass loading. The lower droplet velocity produces longer evaporation times in the flame zone and thus yields the increase in suppression efficiency seen in Fig. 6. Similar observations are also seen for the $50\mu m$ cases but to a lesser extent and are consistent with the modest suppression efficiency rise seen in Fig. 6.

In summary, predictions of suppression efficiency show a strong dependency on drop size. An exploration of drop size on suppression efficiency indicates that an optimum mass loading does occur for the smallest sized $5\mu m$ drops and an increase in suppression efficiency with increasing mass loading for the larger 25 and $50\mu m$ drop cases. The predictions using the drop sizes of this study bound the experimental results for suppression efficiency with the small $5\mu m$ providing too much suppression and the $50\mu m$ drops providing too little. However, even the qualitative trends of suppression efficiency are highly dependent on drop sizes. Therefore it appears that the exact drop size distribution must be well known before quantitative comparisons can be made with confidence.

CONCLUSIONS

A spray-suppression model has been developed for application to turbulent combustions flows of engineering interest. This model accounts for both the thermal and chemical physical effects of a liquid spray. Calculations were performed to predict the suppression efficiency of an H_2 - air turbulent diffusion flame using water spray. The results show that the suppression efficiency of this flame is highly dependent on the initial drop size distribution of the suppressant. Predictions indicate that smaller droplets show an optimal suppressant efficiency while larger drops show an increase in efficiency with increasing mass loading for the ranges of mass loading considered. Results from this work suggest that detailed measurements of drop sizes are needed in suppression studies to allow for even trend analysis of spray-suppression models.

ACKNOWLEDGMENT

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Table 1. Spray source term contributions accounting for non-evaporation (Sd^*) and evaporation (Sd^{**}) for two-way coupling to gas phase. Total spray source term, $Sd = Sd^* + Sd^{**}$. Details of terms in the table can be found in Eq.(1).

Gas phase equation	Non-evaporating source terms, Sd^*	Evaporating source terms, Sd^{**}
Mass	0	$-\frac{1}{V_c} \sum_1^{N_d} \dot{m}_d$
Momentum	$-\frac{1}{V_c} \sum_1^{N_d} (F_{Dj} + F_{bj})$	$-\frac{1}{V_c} \sum_1^{N_d} \dot{m}_d u_{dj}$
Energy	$-\frac{1}{V_c} \sum_1^{N_d} \dot{Q}_{dc}$	$-\frac{1}{V_c} \sum_1^{N_d} \dot{Q}_{de}$

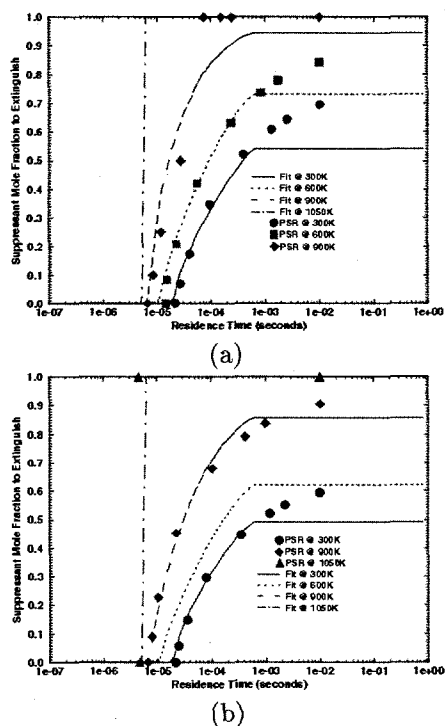


Figure 1. Blowout suppressant mold fraction vs. residence time for stoichiometric H_2/air mixtures with (a) N_2 (in excess of air) and (b) H_2O suppressants at 1 atm pressure. Symbols are from PSR-CHEMKIN calculations and lines are curve fits.

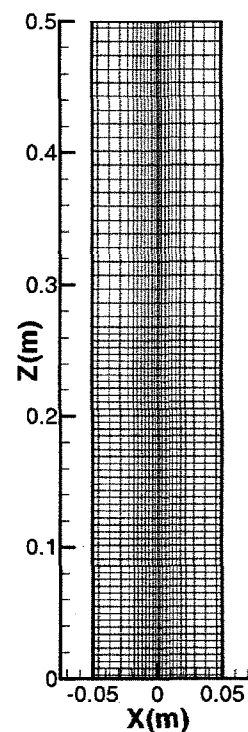


Figure 2. Grid used for suppression problems.

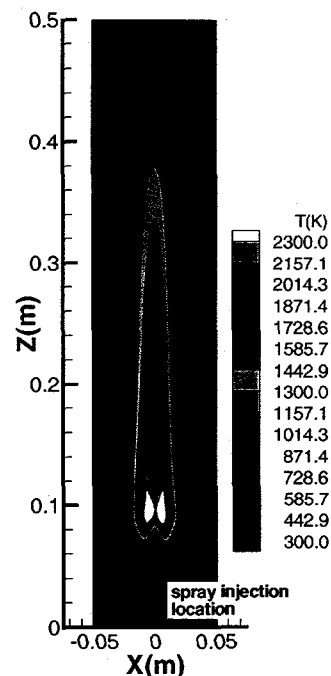
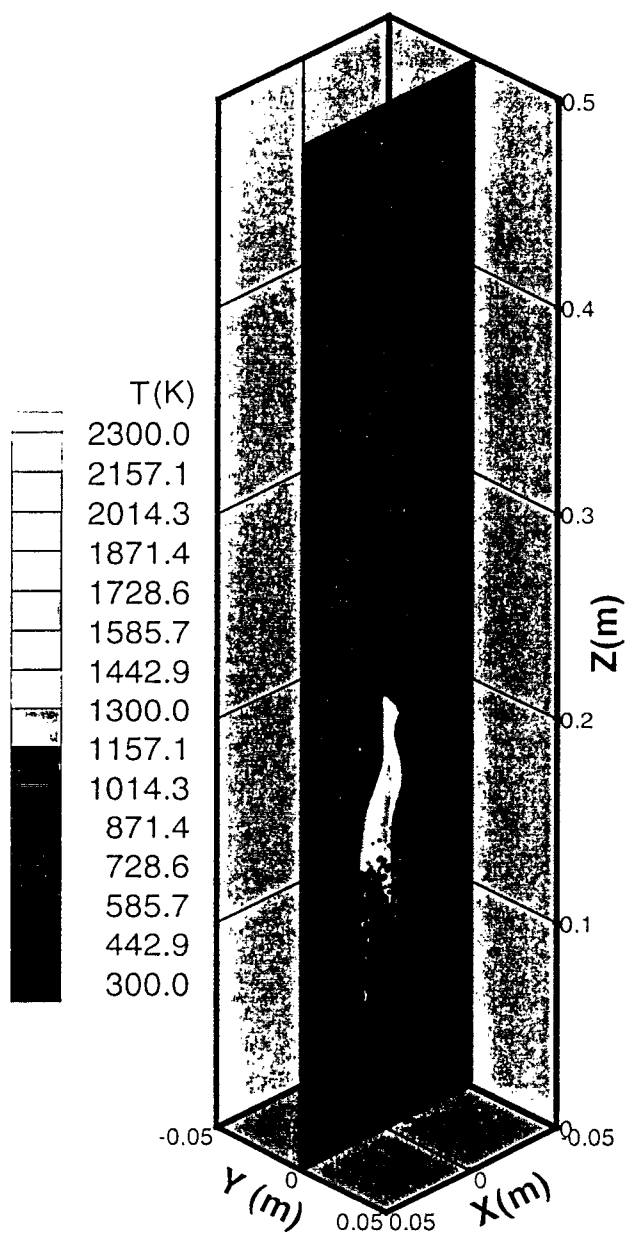
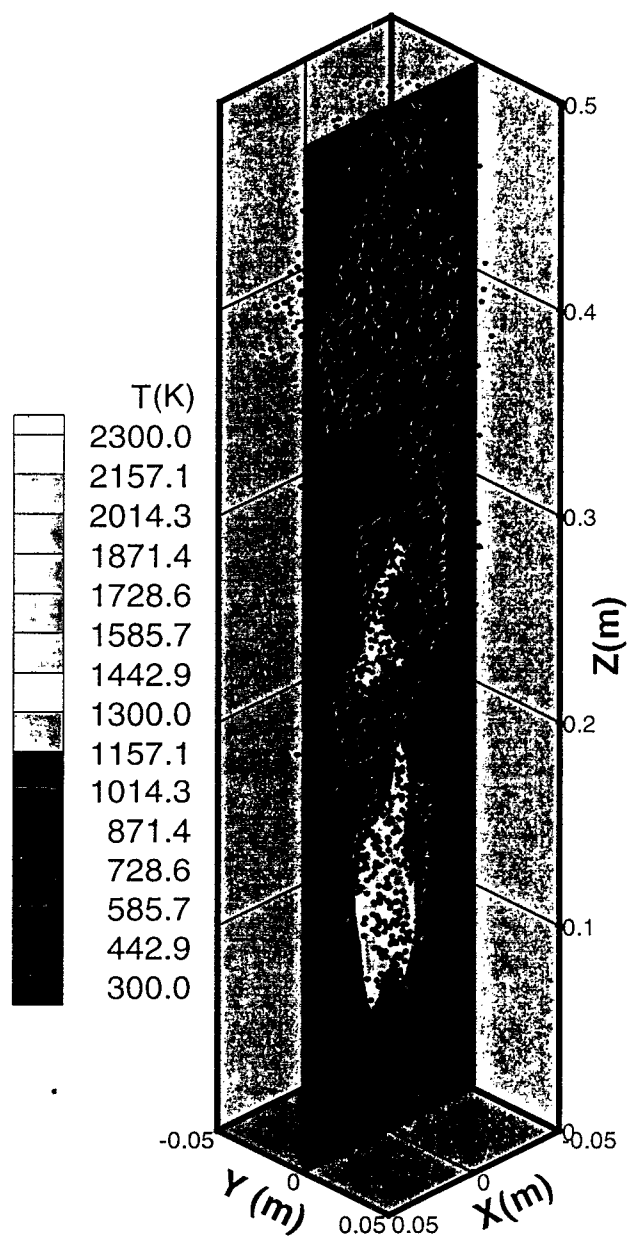


Figure 3. Temperature contours of lifted $H_2 - air$ flame from computation without spray.



(a)



(b)

Figure 4. Instantaneous snapshot of gas phase temperature and spray parcel positions for the $\dot{m}_{H_2O}/\dot{m}_{H_2} = 5$ spray suppression case using (a) 5μm and (b) 50μm drops.

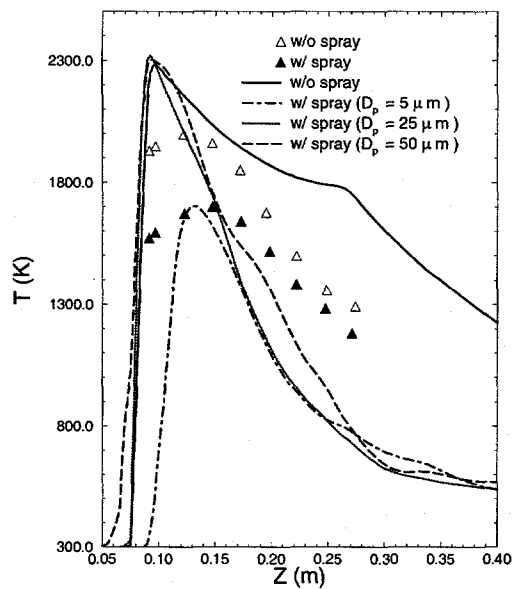


Figure 5. Comparison of temperature vs. streamwise distance.

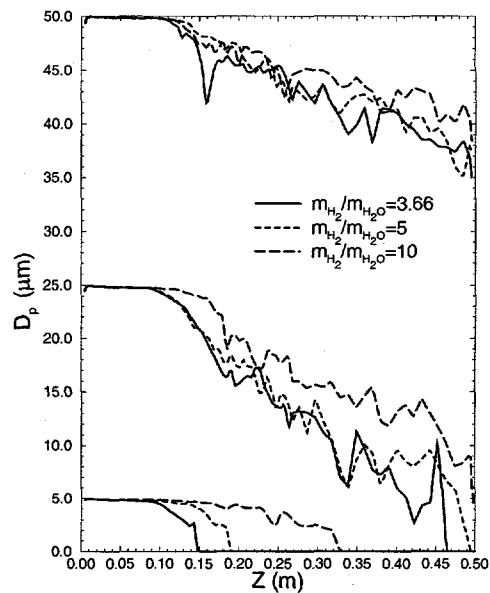


Figure 7. Centerline comparisons of $\overline{D_d}$ vs. Z .

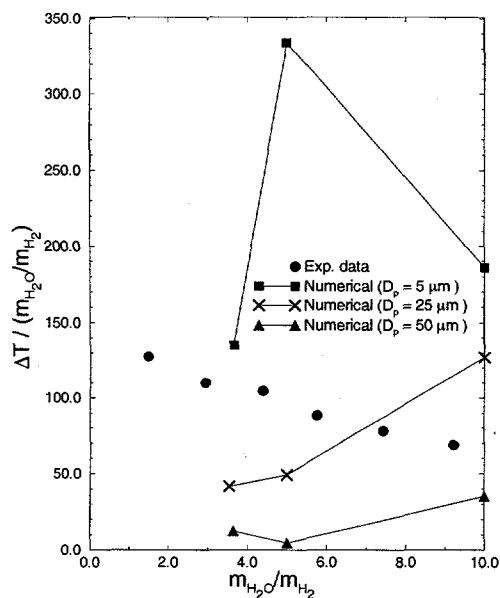


Figure 6. Comparisons of $\Delta T / (\dot{m}_{H_2O} / \dot{m}_{H_2})$ at the centerline and for $Z = 0.122m$.

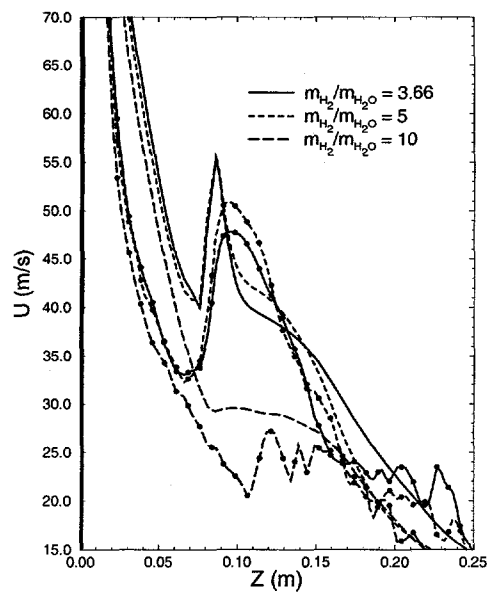


Figure 8. Centerline comparisons of $\overline{U_d}$ (line w/ symbols) and $\overline{U_g}$ (line w/o symbols) vs. Z using the $25\mu m$ drops.

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