

# MODELING THE EFFECT OF WATER SPRAY SUPPRESSION ON LARGE-SCALE POOL FIRES

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## ABSTRACT

In practical fire suppression systems for large rooms or compartments, water sprinklers are often located on or near the ceilings. In this configuration, the droplets from the water spray must be large enough to penetrate the high temperature thermal plume of the fire and reach the pool surface, yet be small enough to evaporate and provide effective suppression of the flame zone. The focus of this research is to investigate computationally the influence of initial drop size and spray system configuration on water suppression of medium to large scale (i.e., ~100kW) pool fires. The cases addressed are representative of ongoing experiments at the Naval Research Laboratories. The fire scenario examined in this study involves a 123kW heptane pool fire located in a 3.05m (10 ft) cube enclosed facility. Results from this study indicate that (1) for large drops ( $D_d > 150\mu\text{m}$ ) an initial rise in temperature is observed associated with enhanced turbulent mixing before evaporative cooling takes place; (2) an optimum drop size is found that allows for maximum decrease in gas-phase temperature for one of the spray configurations examined; and (3) a low pressure spray with more nozzle locations appears to provide improved suppression when compared to using a single high pressure nozzle.

## INTRODUCTION

The purpose of this research is to explore the use of numerical modeling for simulation of fire suppression using water sprays. This capability is useful to assess the performance of halon alternatives as driven by the ban on halon production. One attractive alternative for halon is the use of 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 for fire suppression can be found in the reviews by Tatem et al. [1], Jones et al. [2], Mawhinney et al. [3], and Grant et al. [4]. More recent numerical studies in this area can be found in the works of Chow et al. [5], Novozhilov et al. [6], and Prasad et al. [7, 8, 9]. 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 [7, 8] and pool fires [9]. 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 upward through the base of the flame. These conclusions are also supported in the work of Novozhilov et al. [6] and Chow et al. [5] for enclosure fires.

Novozhilov et al. [6] show reasonable agreement with experimental data by only considering the thermal effects of the spray, thus indicating that the chemical effects of water vapor on exothermic reaction kinetics are not significant. Lentati et al. [10] support this idea in their study 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 contribute 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 water spray suppression of a turbulent fire involves resolving the intimate coupling of liquid evaporation, turbulence, finite rate chemical kinetics, and radiation heat transfer. The objective of this work is to account directly for the first three of these physical processes through subgrid modeling of pool fires for a scenario of engineering interest.

A detailed description of the subgrid models developed to account for thermal cooling (spray submodel) and chemical kinetics effects (PSR submodel) is provided in the Mathematical Model Formulation section. Results are then presented for a square (0.305 m [12 in]) 123 kW heptane pan fire, which is representative of tests at the Naval Research Laboratory (NRL) [11].\* Numerical predictions are presented to examine the sensitivity of volume averaged temperature in the test cell to initial drop size specification and suppression system configuration.

## MATHEMATICAL MODEL FORMULATION

The following mathematical description is limited to a summary of the spray and flame extinguishment model formulations used 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 [12]. VULCAN uses a RANS based model suite including a k-ε turbulence model [13], the EDC combustion model [14], a soot model [15], and a radiation model [16]. 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 [17]. Previous studies using VULCAN for pool fire simulations can be found in references [18, 19, 20].

### SPRAY SUBMODEL

The spray submodel is based on a stochastic separated flow approach [21]. The following transport equations for mass, momentum, and energy are integrated in time for groups of droplets (parcels).

$$\begin{aligned} \frac{dm_d}{dt} &= \pi D_d \rho_f \frac{v_f}{Sc_f} B_m Sh_f \\ m_d \frac{du_{d_i}}{dt} &= \frac{1}{8} \rho_g D_d^2 C_D |u_{g_k} - u_{d_i}| (u_{g_j} - u_{d_j}) + gm_d \delta_{3j} \\ m_d C_d \frac{dT_d}{dt} &= \pi D_d \rho_f \frac{v_f}{C_{p_f}} Pr_f (T_g - T_d) Nu_f - \dot{m}_d h_{lg} \end{aligned} \quad (1)$$

In Eq. (1), the Sherwood ( $Sh_f = h_{m_d} D_d / D_{m_j}$ ) and Nusselt ( $Nu_f = h_d D_d / k_f$ ) transfer numbers are expressed in terms of film conditions using the Ranz-Marshall correlations [22],

$$\begin{aligned} Sh_f &= 2 \log(1 + B_m) / B_m \left[ Re_d^{1/2} Sc_f^{1/3} / 3 \right] \\ Nu_f &= 2 \log(1 + B_m) / B_m \left[ Re_d^{1/2} Pr_f^{1/3} / 3 \right] \end{aligned} \quad (2)$$

\* Maranghides, A., Anleitner, R.L., Binnette, C., Austin, E.M. and Sheinson, R.S., *Results for Self-Contained Total Flooding Halon 1301 Alternative Technologies Evaluation*, NRL report. In progress, 2000, draft on file with the author.

The coefficient of drag ( $C_D$ ) is modeled as that of a sphere using the relations from Shuen et al. [23],

$$C_D = \begin{cases} 24(1 + \text{Re}_d^{2/3}/6)/\text{Re}_d & \text{for } \text{Re}_d < 1000 \\ 0.44 & \text{for } \text{Re}_d > 1000 \end{cases} \quad (3)$$

The thermodynamic properties at the droplet film surface are obtained by using a thin-skin approximation [21] 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,

$\alpha = \text{MIN}(C_{Bi} Bi, 1)$  where  $Bi (= h_d D_d / k_f)$  is the thermal Biot number. The model constant  $C_{Bi}$  (set equal to 0.5) defines the transition  $Bi$  number for which the droplet can be treated using a lumped capacitance approach (i.e.,  $T_d \cong T$ ). This model is used to account for rapid changes in droplet temperature as the droplet is transported into a flame zone. Attempts to use a simple 1/3 rule weighting [24] results 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,  $P_f = P_{ref} \text{Exp}[-h_{lg} / R(1/T_f - 1/T_{ref})]$  where heat of vaporization,  $h_{lg}$ , is expressed as a function of temperature using Watson's relation [25, 26] (i.e.,  $h_{lg} = h_{lg,ref} [(T_c - T_f)/(T_c - T_{ref})]^{0.38}$ ). Once the partial pressure is determined, the mass fraction of water vapor is calculated from the ideal equation of state,  $Y_w = MW_{H_2O} / MW_g (P_g / P_f - 1 + MW_{H_2O} / MW_g)$ . Lastly, the mass ( $B_m$ ) and thermal ( $B_T$ ) transfer numbers in Eq. (1) are obtained from their definitions as derived from steady-state droplet analysis [27]:  $B_m = (Y_g - Y_f) / (Y_f - 1)$  and  $B_T = C_{p_f} (T_g - T_f) / h_{lg}$ .

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 [28] as modified by Shuen et al. [23]. Turbulent dispersion of the droplets within a parcel is accounted for using the group modeling concept of Zhou and Yao [29] where the spatial distribution of droplets within each parcel is 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 subgrid model was developed based on Perfectly Stirred Reactor (PSR) theory as formulated by Glarborg et al. [30] in the CHEMKIN II [31] 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  $H_2O$ ,  $CO_2$ ,  $N_2$ , 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 that allow the mixture mole fraction of suppressant to be determined using the following expression from Saito et al. [32]:

$$\frac{1}{X_{LIM\ mixture}} = \sum_{species} \left( \frac{X_{relative}}{X_{LIM\ species}} \right) \quad (4)$$

where  $X_{LIM\ species}$  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 [32] 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 Figures 1a and 1b. 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 representative curve fits. Mixtures of  $H_2O$  and  $N_2$  are treated using the results of Figure 1 and the mixing rules of Eq. (4). 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 employs 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  $t_{flow} < Da_{crit} t_{PSR}$ , then blowout is assumed to occur and the reaction rates in the EDC combustion model are set equal to zero. The calibration parameter,  $Da_{crit}$ , for the model is the critical Damkohler number for extinguishment and is calibrated from jet blowoff studies" to a value of 1.367. A similar criteria for flame extinguishment has been recently used by Koutmos [33] for LES, but  $Do_{,,,}$  comes from a dynamic length scale ratio rather than an assumed constant. More details on the PSR flame extinction model formulation and its calibration can be found in the reference of Tieszen and Lopez.<sup>\*</sup>

## NUMERICAL IMPLEMENTATION

The droplet transport equations of Eq. (1) are numerically integrated using the LSODE package for solving systems of stiff ODEs [34]. Gas phase properties needed for the evaluation of droplet transport processes are determined using linear interpolation from the Eulerian grid of the CFD calculations. As a first step, droplets that impact any wall of the computational domain before evaporating are simply removed from the calculation allowing a rather conservative prediction of suppression (i.e., dilution of the liquid fuel due to water spray is not modeled). The effects of the spray are coupled to the gas phase equations through appropriate source terms in the gas phase transport. The source terms are integrated into the gas phase transport equations using a dynamic time-splitting subcycling procedure similar to Amsden [35] to provide numerically stable solutions for rapidly evaporating sprays.

<sup>\*</sup>Tieszen, S.R., and Lopez, A., "Development of a Subgrid Fire Extinguishment Model," Technical report. Sandia National Laboratories, Albuquerque, NM. In final preparation, 2000. Draft on file with the author.

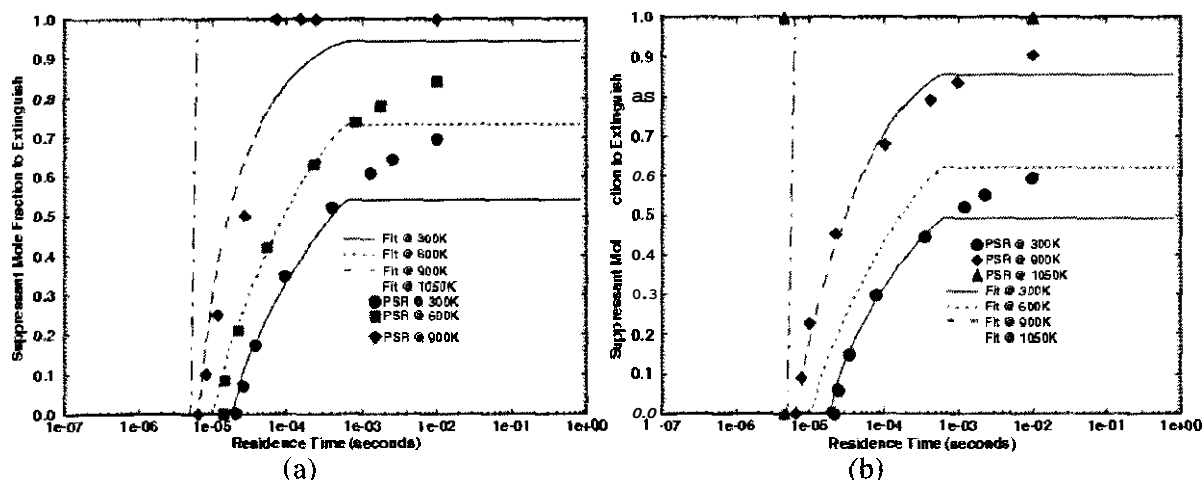


Figure 1. Blowout suppressant mole fraction vs. residence time for stoichiometric  $H_2/air$  mixtures with (a)  $N_2$  (in excess of air) and (b)  $H_2O$  suppressants at 1 atm pressure. Symbols are from PSR-CHEMKIN calculations and lines are curve fits.

The VULCAN simulations presented here employ a  $34 \times 30 \times 37$  grid to discretize a cubical enclosure with a length of 3.05 m (10 ft) on a side. The simulations are first performed for 8600 time steps to simulate 45 sec of physical time to account for a typical preburn time for a fire to ignite and develop. The calculations are then advanced another 3500 time steps to allow for simulation of 10 sec of physical time to elapse with the water suppression activated. During the transient period of spray injection, a total of 33,000 computational parcels are injected into the domain with approximately 2000 parcels at any given time in the simulation.

## RESULTS

A sketch of the NRL test facility is shown in Figure 2. The facility is ventilated using one inlet port located near the top of the enclosure and two exit ports located on the opposite corner. The volumetric flow rate is maintained at  $7.1 \text{ m}^3/\text{sec}$  allowing for one air exchange every 4 min. A  $0.305 \text{ m}$  (12") square pool of heptane is simulated through constant mass flux boundary conditions at the bottom of the domain. The mass flux is chosen as  $\dot{m}'' = 0.0288 \text{ kg}/\text{m}^2 - \text{sec}$  based on empirical correlations from Drysdale [36] (i.e.,  $\dot{m}'' = \dot{m}''_{\infty} (1 - \exp(-k\beta D))$ ) where for heptane  $\dot{m}''_{\infty} = 0.101$  and  $k\beta = 1.1$ ) resulting in a 123-kW fire. In attempt to reproduce conditions from existing experimental procedures at the facility, a constant mass flow condition is imposed on the inlet boundary while a constant pressure condition is used at the outflow boundaries. After 45 sec, a constant pressure condition is imposed on both the inlet and outlet boundaries to simulate deactivation of the ventilation system. Two spray configurations, representative of the systems currently employed at NRL, are considered in this study and are illustrated in Figure 3. The first consists of a single high-pressure spray nozzle located at the center top of the enclosure while the second uses four lower pressure nozzles that cover each quadrant of the cell. Unfortunately, the exact drop size and velocity distributions, as well as the spray distribution pattern, are not well known and could not be obtained from the system manufacturers. Based on estimates of the operating pressures and atomizer cross sectional areas, the same mass flow rate,  $0.53 \text{ kg}/\text{sec}$ , was determined for both systems and droplet velocities of 166 and 83 m/sec for Configurations 1 and 2, respectively were calculated. The spray injection is modeled as a solid cone spray that randomly injects computational parcels to cover the specified solid angle. The

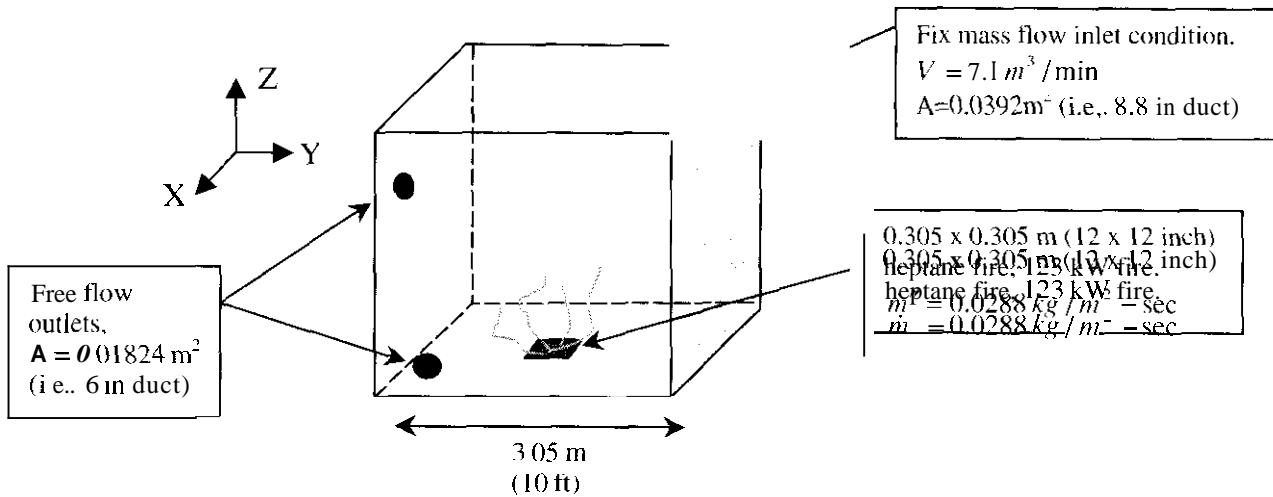


Figure 2. Schematic of NRL test facility.

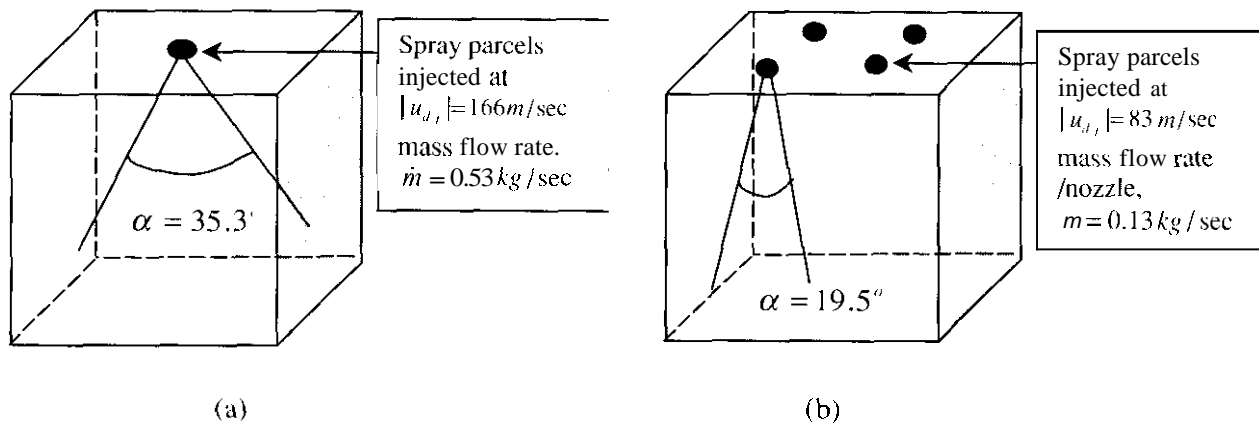


Figure 3. Schematic of spray system configurations using (a) one single high pressure nozzle (Configuration 1) and (b) quadrant approach using four lower pressure nozzles (Configuration 2).

spray angles ( $\alpha$ ) are computed to allow for a spray to reach the corners of the room in Configuration 1 or a cell quadrant in Configuration 2, if the droplet were to follow an outermost trajectory and are set equal to 35.3 and 19.5 deg, respectively. Lastly, four different drop size classes of  $D_d = 25.75, 150$  and  $300 \mu\text{m}$  are used for each configuration to explore the sensitivity of drop size and cover the range of plausible drop sizes expected in the experiments.

Figure 4a shows the volume averaged gas temperature for the lower half (i.e.,  $Z < 1.5 \text{ m}$ ),  $\langle T_l \rangle$ , upper half (i.e.,  $Z > 1.5 \text{ m}$ ),  $\langle T_u \rangle$ , and for the entire domain,  $\langle T \rangle$ , during the preburn part of the simulation. As shown,  $\langle T_u \rangle$ , rapidly increases by approximately 100K in the first 30 sec of the preburn as the hot gases from the pool fire collect near the ceiling of the enclosure. After 30 sec, all temperature averages appear to increase approximately linearly at the same rate of 2 K/sec.

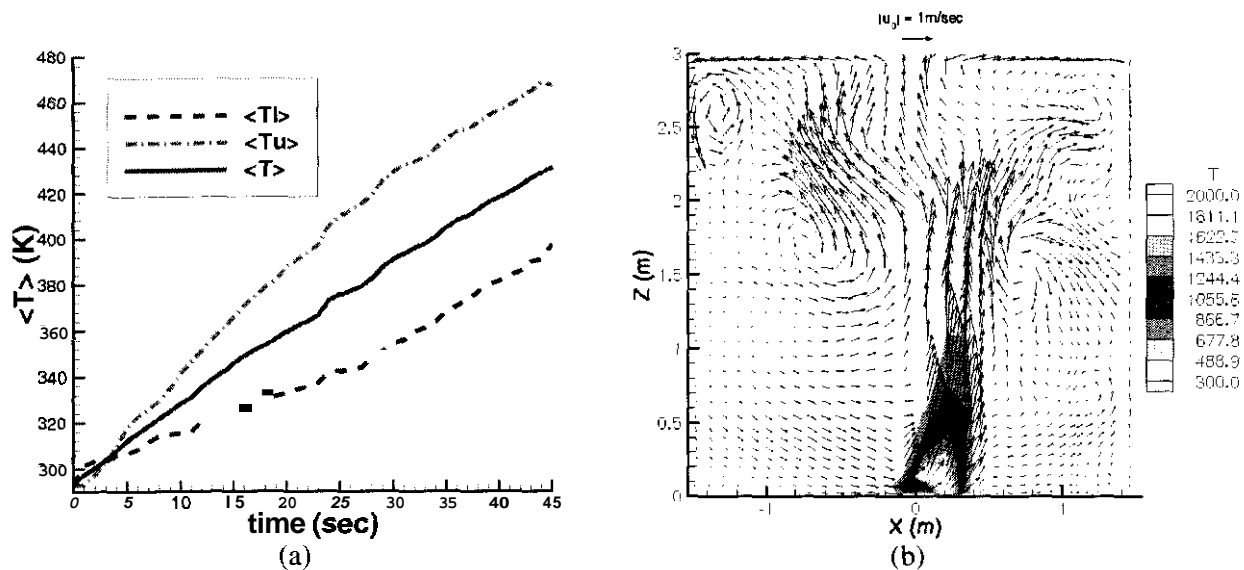


Figure 4. Temperature variations during preburn showing (a) volumetric average temperature versus time during preburn and (b) instantaneous snapshot of temperature isocontour slice through center of cell (i.e.,  $y=0$ ) with superimposed velocity vectors after 45-sec preburn.

Figure 4b shows temperature isocontours with velocity vectors superimposed for a cross section through the domain after the preburn period. At this time, the flow shows large vortical flow structures that entrain air due to the periodic varicose puffing mode of the pool fire. In addition, the location of the peak temperature is shifted toward the outflow boundary resulting in the high temperature gases flowing on average along the ceiling to the exit boundary on the opposite wall.

After the preburn time, the water spray is injected forming a jet of entrained hot gas near the ceiling as the local air is transported by droplet drag and directed downward. Figure 5 shows instantaneous predictions of the gas phase velocity at the spray injection planes along with location and velocity of the droplets after 0.4 sec of spray injection using  $150\mu\text{m}$  droplets for (a) Configuration 1 and (b) Configuration 2. The maximum magnitude of the gas phase velocity for Configuration 2 is approximately 15 m/sec and is about half the peak value of 30 m/sec for Configuration 2. This difference is due to the lower mass flow and associated lower droplet injection velocities for the lower pressure four-nozzle system in Configuration 2.

Figure 6 presents volume averaged temperatures after the start of spray injection for Configuration 1 using all four drop size classes showing (a)  $\langle T_i \rangle$  and (b)  $\langle T_u \rangle$ . In Figure 6a, the largest,  $300\mu\text{m}$ , drops show an initial increase in temperature for the first 2.5 sec after injection. This surprising increase in temperature is due to the enhanced turbulent mixing of the jet and advection on the pool surface before enough water has evaporated to start to cool the flow near the base of the fire. This prediction is consistent with previous observations of Atreya et al. [37] on the use of water sprays. In contrast, the injection of the  $25\mu\text{m}$  drops results in a sudden drop of 40 K in the average temperature near the base of the fire in the first second, leveling off for another 3 sec and then suddenly decreasing again. This temperature history can be attributed to the transient jet development. A high concentration of small droplets are located at the leading edge of the jet offering effective suppression of the pool fire for a short (1 sec) period followed by enhanced turbulent mixing that slows the suppression until the initial jet transient has passed at 48 sec. The intermediate, 75 and  $150\mu\text{m}$ , cases also show signs of the transient jet develop-

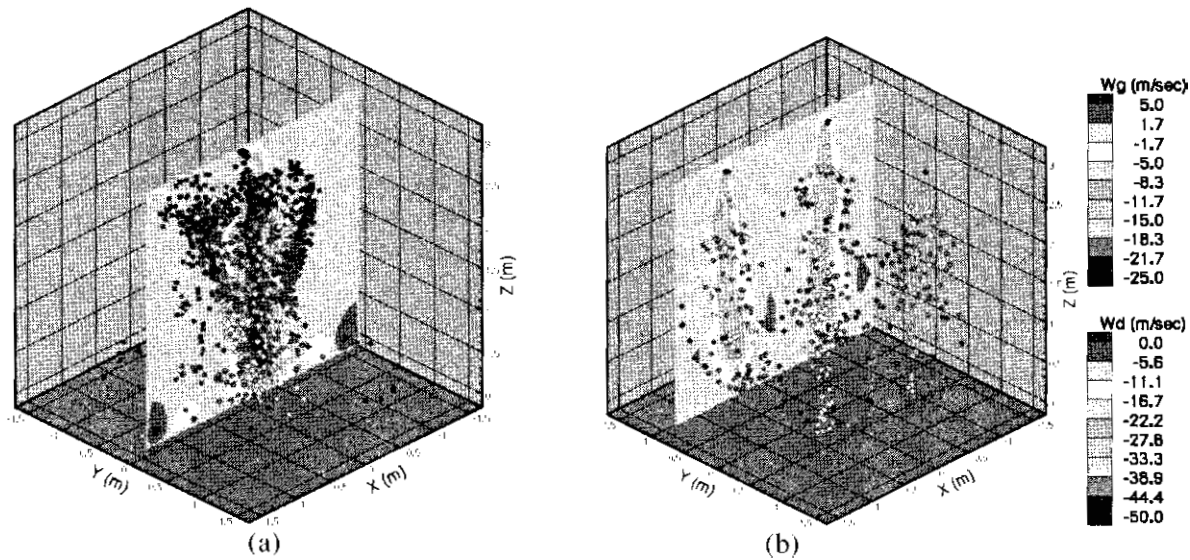


Figure 5. Instantaneous snapshot of water spray suppression 0.4 sec after injection showing isocontours of gas and droplet phase vertical velocity at plane of injection for (a) spray configuration 1 (contour slice at  $y=0.0$  m) and (b) spray Configuration 2 (contour slice at  $y=-0.8$  m).

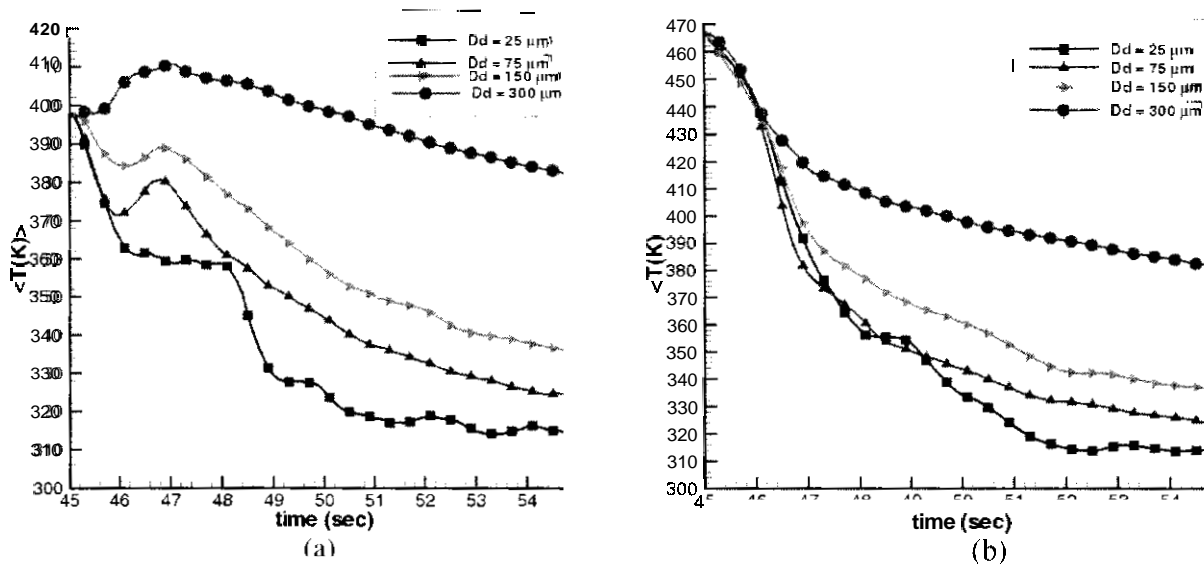


Figure 6. Volume averaged temperature for Configuration 1 showing (a)  $\langle T_l \rangle$  and (b)  $\langle T_u \rangle$  verses time.

ment with some short-lived reduction in temperature due to initial injection of drops followed by an increase in temperature and then a more gradual decrease. Figure 6b shows  $\langle T_u \rangle$  time history and indicates that, in general, the smaller droplets allow for more effective suppression than larger drops with the 25 and 75  $\mu\text{m}$  providing almost same initial reduction in  $\langle T_u \rangle$  for the first 4.5 sec after injection.

Figure 7 show (a)  $\langle T_l \rangle$  and (b)  $\langle T_u \rangle$  time history for the second spray system configuration. In this case, the enhanced turbulent mixing due to the startingjet from the sprays is not as pronounced as in Configuration 1 due to the lower injection velocities of the droplets and the spatial



offset of the spray injection locations relative to the position of the pool fire. The decrease in turbulent mixing, along with the longer residence time of droplets to interact with the fire, allows for the spray in Configuration 2 to decrease the  $\langle T_u \rangle$  temperature more quickly than in configuration 1 as shown by comparing Figure 7b to 6b. In addition, Figures 7a and 7b indicate an optimum drop size exists between 25 and 75  $\mu\text{m}$  that is sufficiently large to penetrate the high temperature fire plume, yet be small enough to be an effective suppressant at the flame zones. This observation is consistent with the previous water spray suppression studies of pool fires [4].

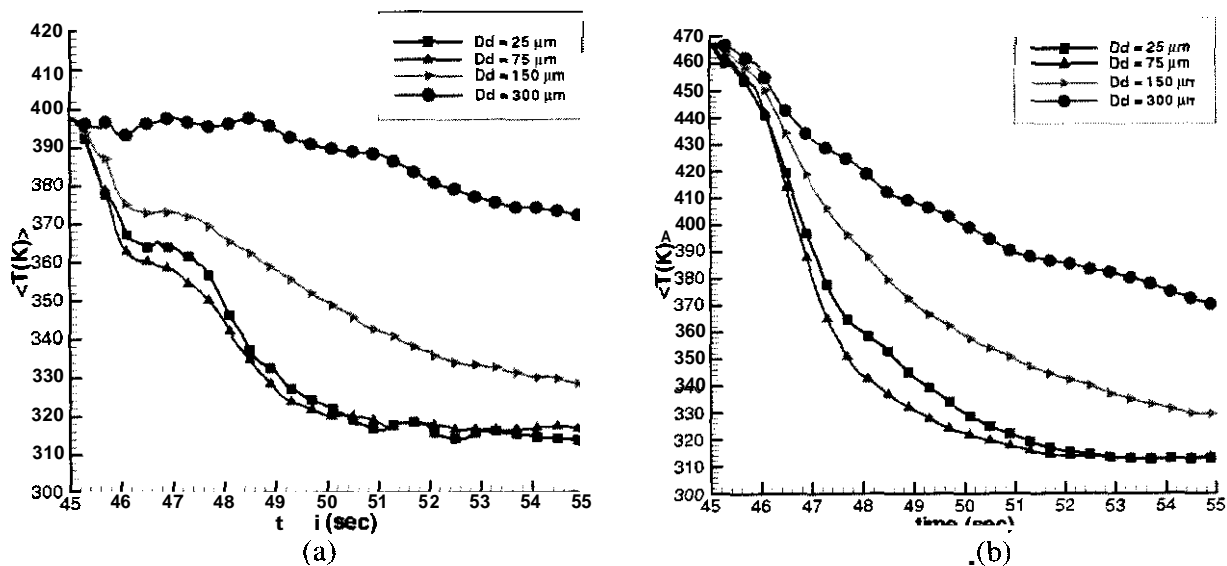


Figure 7. Volume averaged temperature for Configuration 2 showing (a)  $\langle T_l \rangle$  and (b)  $\langle T_u \rangle$  versus time.

## CONCLUSIONS

In summary, a spray-suppression model applicable to simulating the effects of water mist on large-scale pool fires has been developed and applied to a practical fire scenario representative of experiments at NRL. The findings from this study indicate a strong sensitivity of fire suppression to initial drop size where injection of larger drops may actually cause an increase in overall temperature due to enhanced turbulent mixing before enough spray can evaporate to provide sufficient cooling. In spray Configuration 2, an optimum drop size was observed indicating that nozzles that generate very fine mist (i.e.,  $D_d < 50 \mu\text{m}$ ) will not always provide maximum suppression for these conditions. Lastly, within the assumptions imposed for the inlet spray conditions and the fire scenario studied, the spray configuration using several lower pressure nozzles appeared to be slightly more effective at decreasing the gas phase temperature shortly after spray injection than a single high pressure nozzle.

## ACKNOWLEDGMENTS

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