NIST Sponsored Research in Sprinkler Performance Modeling

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Introduction

Rapidly changing building designs, uses, materials, contents, fire protection and the general intermix of industrial/commercial and residential occupancies has created a need to understand the potential hazards and losses from fires and the performance of fire protection systems under conditions that may not be specifically addressed by historic fire testing and codes. In the absence of an accurate understanding of potential fire events, excessively conservative decisions may be made, usually increasing costs and creating barriers to innovation. It is impractical, and in many cases too hazardous, to physically test all fire scenarios of interest.

In cooperation with industry, a numerical fire model, Fire Dynamics Simulator, is being developed at NIST to evaluate the performance of fire protection systems in buildings. The model has been used to generate predictions of fires in industrial facilities protected entirely or in part by automatic fire sprinklers. The heart of the model is a Large Eddy Simulation (LES) based fire model with the capability of simulating large scale industrial fires. Because the model provides far more detailed simulations than zone models can, it requires more detailed information about the fuels, building materials and fire protection systems. The Building and Fire Research Laboratory at NIST has supported efforts, both internally and through its grants program, to develop measurement techniques to generate this information. These measurements include droplet size distributions, spray patterns, droplet trajectories, and heat transfer coefficients. The results of these studies will be used as input to the model so that realistic sprinklers systems can be evaluated.

Improvements to Fire Dynamics Simulator

Version 2.0 of the Fire Dynamics Simulator (FDS2) was publicly released in December 2001 [1, 2]. FDS v2 contains better combustion and radiation routines than the original version, allowing for a gradual improvement in the treatment of the water droplets. Experimental work over the past few years is steadily contributing to a database of information about sprinkler activation [3], spray patterns [4], droplet size [5] and suppression [6]. Still, important physical phenomena associated with droplet behavior have not been implemented in FDS until now because the simplified combustion and radiation routines of FDS version 1 did not support the enhanced physics governing the water droplets. In the present paper, some of these phenomena will be discussed and some sample calculations presented.

Droplet Evaporation

The original version of FDS (version 1) handled droplet evaporation in a very simple way. Hot gases heated the droplets through convection alone. Once the droplets reached the boiling temperature of water, they would evaporate but the water vapor would not be tracked. In some sense, the water simply disappeared from the calculation. This simplification worked reasonably well for large drop sprinklers, but in the case of a mist system, a more detailed description of droplet evaporation is needed. In this section, the evaporation mechanism is discussed. In the next section, absorption of thermal radiation by water droplets will be discussed.

The evaporation of water droplets is handled semi-empirically. A water droplet suspended in air will evaporate as a function of the droplet equilibrium vapor mass fraction, the local gas phase vapor mass fraction, the heat transfer to the droplet, and the droplet's motion relative to the gas. A correlation for the mass loss rate of a droplet that involves these parameters is given here [7]

$$\frac{dm_d}{dt} = -2\pi\, r_d\, \mathrm{Sh}\, \rho D\, (Y_d - Y_g) \tag{1}$$

The subscripts d and g refer to the droplet and gas, respectively, ρ is the gas density, r_d is the droplet radius, m_d is the droplet mass, D is the diffusion coefficient for water vapor into air, Y is the water vapor mass fraction, and Sh is the droplet Sherwood number, given by a correlation involving the Reynolds and Schmidt numbers

$$\mathrm{Sh} = 2 + 0.6\, \mathrm{Re}^{\frac{1}{2}}\, \mathrm{Sc}^{\frac{1}{3}} \tag{2}$$

The vapor mass fraction of the gas, Y_g, is obtained from the overall set of mass conservation equations and the vapor mass fraction of the droplet is obtained from the Clausius-Clapeyron equation

$$X_d = \exp\left[\frac{h_v\, M_w}{\mathcal{R}}\left(\frac{1}{T_b} - \frac{1}{T_d}\right)\right] \quad ; \quad Y_d = \frac{X_d}{X_d(1 - M_a/M_w) + M_a/M_w} \tag{3}$$

where X_d is the droplet water vapor volume fraction, h_v is the heat of vaporization, M_w is the molecular weight of water, M_a is the molecular weight of air, $\mathcal{R}$ is the gas constant, T_b is the boiling temperature of water and T_d is the droplet temperature.

In addition to calculating the mass transfer due to evaporation, the transfer of energy must also be calculated. The droplet heats up due to the convective heat transfer across the surface of the droplet minus the energy required to evaporate water

$$m_d\, c_{p,w}\, \frac{dT_d}{dt} = A_d\, h_d\, (T_g - T_d) - \frac{dm_d}{dt}\, h_v \tag{4}$$

Here $c_{p,w}$ is the specific heat of water, $A_d = 4\pi r_d^2$ is the surface area of the droplet, h_d is the heat transfer coefficient, given by

$$h_d = \frac{\mathrm{Nu}\, k}{2r_d} \quad ; \quad \mathrm{Nu} = 2 + 0.6\, \mathrm{Re}^{\frac{1}{2}}\, \mathrm{Pr}^{\frac{1}{3}} \tag{5}$$

Nu is the Nusselt number, k is the thermal conductivity of air, and the Prandtl number, Pr, is about 0.7 for air. The Sherwood number, Sh, is analogous to the Nusselt number, with the Schmidt number about 0.6 compared to the 0.7 for the Prandtl number.

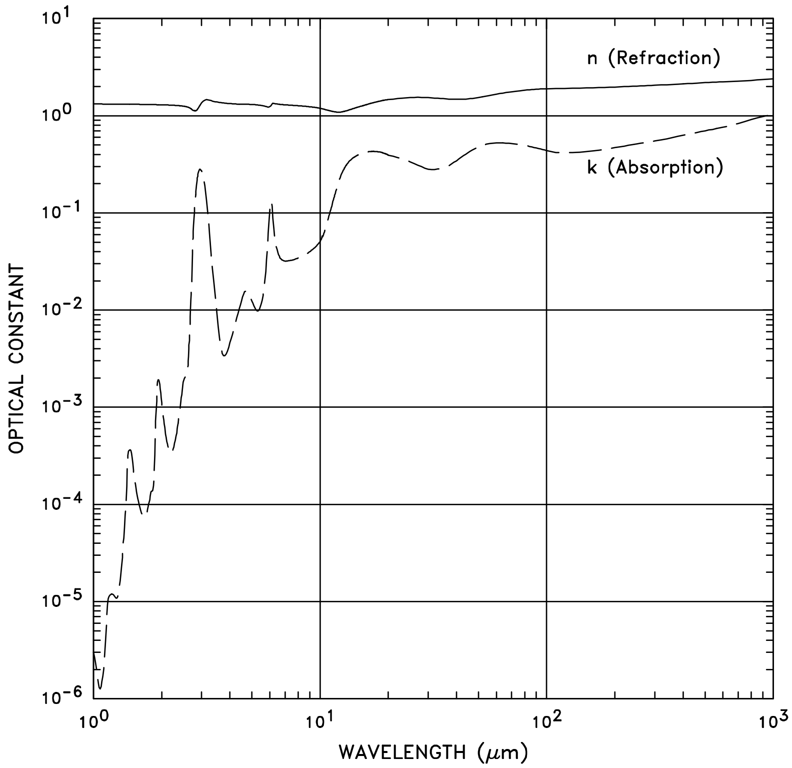

FIGURE 1: Optical constants for liquid water.

Radiation Absorption

The attenuation of thermal radiation by water droplets is an important consideration, especially for water mist systems [8]. Water droplets attenuate thermal radiation through a combination of scattering and absorption [9]. These processes are typically represented by a wavelength dependent complex number, $n + ik$, called the refractive index. In this expression n is the refractive factor of the index, used in Snell's Law to determine the bending of light at a material interface, and k is the extinction coefficient. The refractive index has been measured for a number of materials and is shown in Figure 1 for water [10].

The scattering and absorption processes are functions of the wavelength, the droplet size, and the angle of the ray normal to the surface of the scattering droplet. To calculate the net attenuating affect of a field of droplets in a rigorous manner requires the computationally intensive application of Mie theory or some other scattering/absorption theory. These computations are too expensive for use in FDS, and instead a simpler form is used. A wavelength averaged attenuation constant called the extinction coefficient is calculated as a function of droplet radius. This allows the attenuation of radiation to be calculated [8]

$$\frac{I}{I_0} = e^{-3\,K\,W\,L/4\,r_d\,\rho_w} \quad (6)$$

where I and I_0 are the outgoing and incoming radiant intensities, K is the wavelength-averaged, radius-dependent extinction coefficient, W is the mass of water per unit volume, L is the path-length, r_d is the droplet radius, and ρ_w is the droplet density. Everything except for K is obtained from other parts of the calculation. K is the sum of the scattering, K_s, and absorption, K_a, coefficients for the droplet. These values are determined as follows [11]

$$K_s(\lambda, r_d) = 2\left[1 + \frac{1}{\alpha(n-1)}\left(1 - \frac{\cos(2\alpha(n-1))}{2\alpha(n-1)} - \sin(2\alpha(n-1))\right)\right] \quad (7)$$

$$K_a(\lambda, r_d) = 1 + \frac{2\left(\exp(-4\alpha nk) + (\exp(-4\alpha nk) - 1)/(4\alpha nk)\right)}{4\alpha nk} \quad ; \quad \alpha = \frac{2\pi r_d}{\lambda} \quad (8)$$

where λ is the wavelength and r, n, and k are defined above. The extinction coefficient K can be averaged over the wavelengths of interest to yield a function of the droplet radius only. This approximation is consistent with the gray-gas assumption used in the radiation transport algorithm. In the radiation solver, information on the droplet radii and droplet number density in a grid cell can be used to determine K. The radiation solver then adds the resulting attenuation factor to that calculated for any absorbing gas present in a cell. The radiation energy absorbed by the droplet is then added to the convective heat transferred to the droplet by the hot gases.

Applications

As a simple test of the new droplet evaporation and radiation absorption routines, a simulation is performed of a single sprinkler in the center of a 3 m by 3 m by 3 m compartment. The right hand wall of the compartment is given a prescribed temperature of 1000 °C. Without a sprinkler spray, the center of the left hand wall is exposed to a heat flux of about 60 kW/m^2. With the sprinkler flowing at a rate of 400 L/min (110 gpm), the heat flux is reduced to about 20 kW/m^2. The temperature of the intervening water droplets varies from 65 °C nearest the hot wall, to 20 °C nearest the target cold wall.

A more complex example of the new algorithm is shown in Fig. 2. Here a mist sprinkler system is installed in a simplified machinery space whose dimensions are 16 m by 10 m by 8 m. The 6 MW fire is fueled by a series of heptane spray burners lined along the top of a steel box centered in the compartment. Eight mist nozzles are positioned at the ceiling, 4 m apart. Four nozzles are positioned above the 2 m by 2 m opening centered along the longer wall, 0.5 m above the floor. The nozzles are activated a short time after the ignition of the fuel burners. The small water droplets evaporate due to both the high temperatures in the upper smoke layer, and the absorption of thermal radiation from the fire. The water vapor displaces oxygen and the water evaporation cools the compartment, both of which weaken the fire. The numerical algorithm appears to handle the evaporation and transport of the water vapor, but a problem remains in predicting the change in burning behavior. Presently, the FDS contains a mixture fraction combustion model that assumes an infinitely fast reaction between fuel and oxygen regardless of temperature. Dilution of the air by smoke, exhaust gases and water vapor is predicted in the model, but the unburned fuel due to a lack of oxygen eventually burns somewhere in the compartment, even though the lower temperature in reality would not sustain this burning. Thus, the focus of attention needs to be turned back towards the combustion routine so that the suppression of the fire in an underventilated space can be handled better. Even in the absence of a sprinkler system, there is a need to better understand the weakening of a fire in an underventilated compartment.

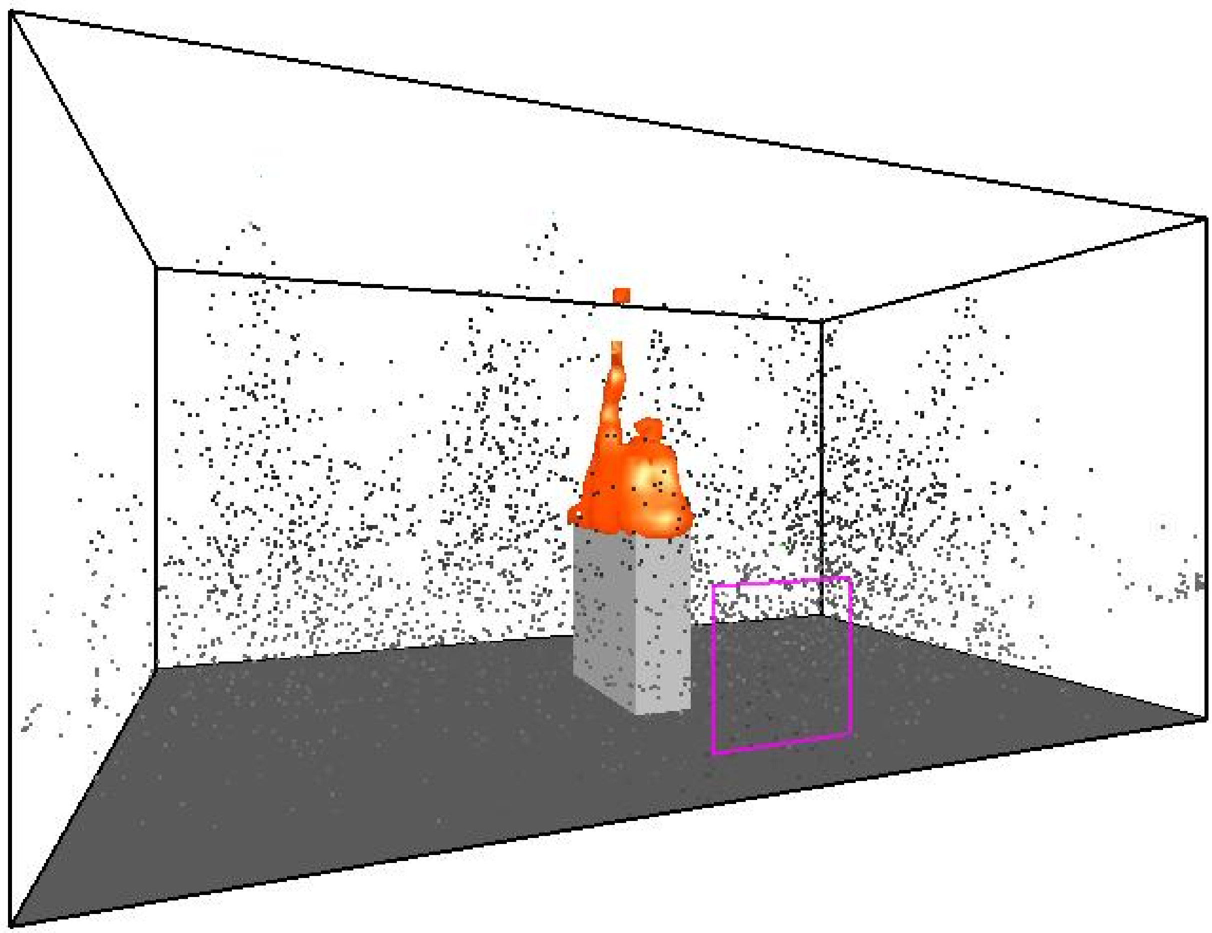

FIGURE 2: Simulation of a mist system suppressing a large heptane spray burner fire. Shown is the outline of the flame and the water droplets.

Liquid Fuel Combustion

A substantial part of the internal program of the Building and Fire Research Laboratory at NIST has been re-directed towards an analysis of the fire and collapse of the World Trade Center on September 11, 2001. As part of this effort, FDS is being used as a simulation tool to re-create various aspects of the fire. A few of the algorithms built into FDS to handle sprinkler sprays have proven useful in other areas, especially in treating the burning of liquid fuels, both liquid pools and liquid droplets. Following is a brief description of a few ongoing projects in which the evaporation and absorption routines described above are being used elsewhere.

Methanol Pool Fires The burning of a pool of liquid fuel has been studied a great deal not only because many accidental fires involve the burning of spilled liquids, but also because liquid fuel fires can be very well characterized experiments. The burning rate can be measured easily, and if the fuel is an alcohol, the fire is often free of soot and easier to study than a soot-laden fire. Simulations of methanol pool fires were carried out for pools of various diameters ranging from 1 cm to 100 cm. The burning rate of the pool was predicted using the same assumptions used to handle the evaporation of sprinkler water droplets. Figure 3 shows the instantaneous simulated flame shapes for 10 cm and a 30 cm pool. Note that the 30 cm case is more turbulent than the 10 cm. Work is ongoing to predict the burning rate of the fuel based on the heat fed back from the fire to the pool surface. The error in these predictions is substantial because of the uncertainty in the absorption coefficient of the fuel gases, and the lack of adequate grid resolution at the pool surface.

Oil Well Blowout Fires

Oil well blowouts result from a failure in the well or well operations that allow gas and/or oil to escape to the surface. Oil well blowouts are rare and there are safeguards to prevent them. They are most likely to occur during drilling operations and can lead to oil being spread over a significant area. In some cases the oil and gas from a blowout will ignite and in other cases it will not. Preliminary calculations of oil well blowout fires (see Fig. 4) have demonstrated that the jet of flames emanating from an uncapped well head can be modeled with computational cells on the order of 15 cm to 30 cm (6 in to 1 ft), and the numerical grid is then stretched away from the fire to save on CPU time. Transport of the unburned droplets downwind can be handled well on a coarser mesh consisting of cells on the order of several meters. Radiation absorption by the fuel droplets (the same methodology used for sprinkler water droplets) is key to understanding which oil droplets will survive the fire and be blown downwind. In this case, the same physical mechanisms are used to treat the radiation absorption by the fuel droplets, but the properties of crude oil are not as well-characterized as water. Plus, the size and velocity of the oil droplets escaping the well head are not well known. The study is aimed at developing an upper and lower bound on the amounts of liquid fuel consumed in the fire, and the amount escaping the fire.

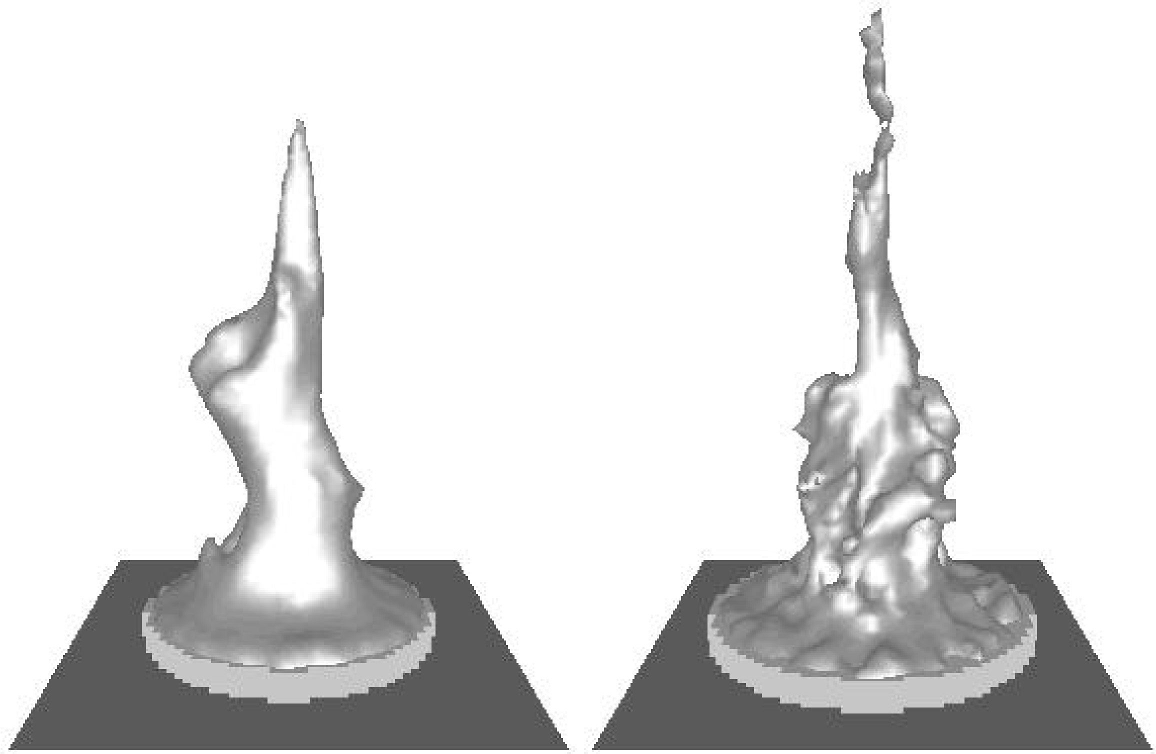

FIGURE 3: Simulation of a 10 cm (left) and 30 cm (right) methanol pool fire.

Conclusions

The development of a numerical model to simulate fire, sprinklers and other fire-related phenomena continues. The latest improvements to the sprinkler algorithm focus on the evaporation and radiation absorption by water droplets. These effects are particularly important for the evaluation of mist suppression systems. As work continues to validate the new routines, some of the physical mechanisms have been found to be useful for other purposes besides water droplets, especially the burning of liquid fuels, both pools and droplets. The events of September 11, 2001, have redirected some of the efforts at NIST to understanding the burning behavior of large pools of liquid fuels and fuel droplets. Increased understanding and new numerical algorithms aimed at the World Trade Center disaster will benefit the sprinkler work since the underlying physical mechanisms are similar.

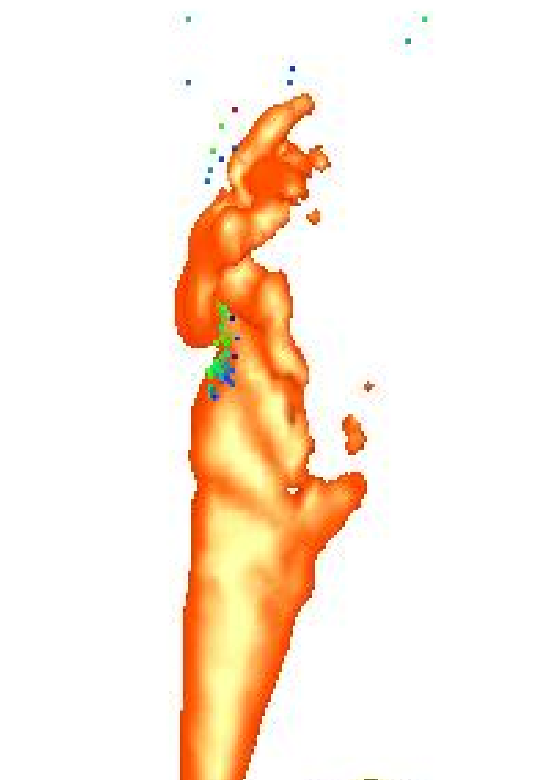

FIGURE 4: Simulation of an oil well blowout fire.

References

[1] K.B. McGrattan, H.R. Baum, R.G. Rehm, G.P. Forney, J.E. Floyd, and S. Hostikka. Fire Dynamics Simulator (Version 2), Technical Reference Guide. Technical Report NISTIR 6783, National Institute of Standards and Technology, Gaithersburg, Maryland, November 2001.

[2] K.B. McGrattan, G.P. Forney, J.E. Floyd, and S. Hostikka. Fire Dynamics Simulator (Version 2), User's Guide. Technical Report NISTIR 6784, National Institute of Standards and Technology, Gaithersburg, Maryland, November 2001.

[3] P. Ruffino and M. di Marzo. Measurements in a hot gas laden with water droplets: gas temperature. *Submitted to the Journal of Heat Transfer*.

[4] P.D. Gandhi, D. Sheppard, and R. Lueptow. Understanding Sprinkler Sprays:. In *Proceedings of the Fire Suppression and Detection Research Application Symposium*. The Fire Protection Research Foundation, Quincy MA, 2000.

[5] J.F Widmann and D. Sheppard. Characterization of a Residential Fire Sprinkler Using Phase Doppler Interferometry. In *Proceedings of the Fire Suppression and Detection Research Application Symposium*. The Fire Protection Research Foundation, Quincy MA, 2001.

[6] A. Hamins and K.B. McGrattan. Reduced-Scale Experiments to Characterize the Suppression of Rack Storage Commodity Fires. Technical Report NIST Internal Report (NISTIR 6439), National Institute of Standards and Technology, Gaithersburg, Maryland 20899, 1999.

[7] N. Cheremisinoff. *Encyclopedia of Fluid Mechanics, Volume 3: Gas-Liquid Flows*. Gulf Publishing Co., Houston, Texas, 1986.

[8] T. Ravigururajan and M. Beltran. A Model for Attenuation of Fire Radiation Through Water Droplets. *Fire Safety Journal*, 15:171–181, 1989.

[9] A. Tuntomo, C. Tien, and S. Park. Optical Constants of Liquid Hydrocarbon Fuels. *Combustion Science and Technology*, 84:133–140, 1992.

[10] D. Segelstein. The Complex Refractive Index of Water. Master's thesis, University of Missouri, Kansas City, 1981.

[11] A. Coppalle, D. Nedelka, and B. Bauer. Fire Protetcion: Water Curtains. *Fire Safety Journal*, 20:241–255, 1993.