NUMERICAL MODELING STUDIES OF THE INFLUENCE OF WATER MISTS ON PREMIXED FLAMES IN MICROGRAVITY

Francine Amon, Wenhua Yang, Robert I. Kee,
J. Thomas McKinnon, and Angel Abbud-Madrid
Colorado School of Mines

ABSTRACT

An investigation of the effect of water mists on premixed flame propagation under reduced-gravity conditions is being conducted to aid in the understanding of the fundamental interactions between **a** flame front and water mist Computer modeling shows that the sensible and latent heats of water, as well as increased water concentration, decrease the speed of a propagating flame. Decreasing mist droplet diameter, given **a** constant water mass fraction, also decreases flame speed. Modeling of the absorption of radiation by water mist droplets shows an increase in the evaporation rates of the droplets, which in turn causes a further inhibiting effect on flame propagation. An understanding of the dynamics of the water mist aerosol **is** necessary to estimate the mist loadings and droplet diameters used as input for the model. A second model is being developed that will track the side distribution and number density of the water-mist droplets for this purpose.

INTRODUCTION

Modeling, in conjunction with experimentation, is being conducted in the interest of expanding the body of knowledge pertaining to the fundamental interactions between fine water mist and fire. Currently, the level of understanding of the relationships between water mist and fire justify full-scale fire testing of water mist fire protection system designs [1]. On the other hand, basic research in this area contributes to a more complete understanding of the principles at work, eventually allowing fire protection engineers to estimate optimum mist droplet size distributions, mist loadings, and fire suppression system configurations with confidence to augment full-scale testing. Most water mist research to date targets specific applications such as pool fires, aircraft-compartment fires, and shipboard machinery rooms. Full-scale fire testing opportunities, for example, of an aircraft cabin [2], do not often occur, although the results of such testing can be quite beneficial. Basic full-scale testing of large uncluttered enclosures with simple geometries provides excellent data against which to compare modeling results [3], but extrapolation to different conditions and configurations is risky at best.

The modeling component of this work falls into two categories: (1) examination of the relative importance of the various fire-suppression mechanisms present when water mist droplets are in contact with a flame, and (2) modeling of the dynamics of the mist aerosol as it exists prior to direct interaction with a flame. In both cases, conditions as specific to the experimental apparatus as possible are imposed so that the models may be calibrated and verified with experimental data. The details of the experimental constraints are discussed in the following section.

EXPERIMENTATION

Experiments have been performed in normal gravity, however, the distorting effects of buoyancy-induced flow patterns, coupled with difficulties in suspending a uniform concentration of mist have led to the need to conduct experiments under microgravity conditions. To this end experiments have been performed in the reduced-gravity environment of **NASA KC-135** aircraft and are scheduled for the Combustion Module (CM- 2) onboard Space Shuttle flight STS-107 (2002) and on the International Space Station.

The experimental apparatus consists of a cylindrical polycarbonate tube with an igniter and gate valve at one end and an ultrasonic atomizer nozzle at the other. The tube is divided at its midsection into two chambers by an iris. In a typical test, the entire tube is filled with a C_3H_8-air mixture. The mixture is given time to become quiescent; then the iris closes and mist is injected into the nozzle portion of the tube. The mist is given time to come to rest, during which time it will undergo coagulation and deposition on the tube wall. Modeling of these activities is explained in the following text. The gate valve and iris then open and the C_3H_8-air mixture is ignited. Photodiode arrays and a video camera record the progress of the flame as it propagates from the dry end of the tube into the misted portion of the tube. A detailed description of the experimental apparatus and testing procedure can be found in the literature [4].*

Tests are performed in which the loading and size distribution of the mist as well as the air/fuel equivalence ratio of the mixture are varied and their effect on laminar flame speed recorded. Standard color video and photodiode data are collected for each of the flames. The space experiments will also include infrared video and temperature data.

A separate experiment, based on the principles of light scattering and designed to measure the mist droplet size distribution and number density as a function of time and axial position, is also being developed in order to characterize the water mist as it exists prior to encountering the flame front. This experiment will be conducted both in normal gravity and aboard the KC-135.

MODELING

FIRE SUPPRESSION MECHANISMS

The effect of droplet diameter, number density, and the major fire suppression mechanisms have been incorporated into a computational model [5]. These mechanisms include heat removal from the vaporization of water, dilution of oxygen and fuel due to volume expansion of vaporizing water, retardation of surface flame propagation due to the wetting of surfaces, and the absorption of radiation by the mist droplets. A discussion of the current progress in the development of this model follows.

The physical problem of interest is to determine how flames propagate through an initially quiescent mixture of fuel, air, and water mist. However, from a computational point of view, it is far more efficient to solve a steady-state problem in a flame-fixed coordinate system. Water droplets issuing from a virtual burner face are assumed to have the same velocity as the fuel/air mixture and to be in equilibrium with the water vapor in the gas (i.e., 100% relative humidity). That is, water vapor is added to the fuel/air mixture to assure that there is no droplet evaporation or condensation at the inlet conditions.

The phenomena of flame suppression in a water mist involve strong, two-way coupling between droplet evaporation and flame propagation. The model solves mass, momentum, and energy conservation equations for the water droplets in a Lagrangian framework and one-dimensional conservation equations in an Eulerian framework to solve for the physics of gas-phase flame propagation. Coupling is achieved through addition of droplet-evaporation related source terms in the PREMIX software [6]. PREMIX is part of the suite of combustion-related programs included in the CHEMKTN software package [7].

As droplets approach a flame they begin to evaporate, releasing water vapor to the gas phase. Since they are readily vaporized, small droplets have difficulty penetrating the flame. Large droplets, however, can often survive through the flame and continue to evaporate in the hot post-flame gases. An important aspect of this investigation is to determine the effect of droplet size and number density on flame extinction, and to understand optimal droplet dispersal in tire suppression systems. The propagation speed of a CH_4-air flame is shown (Figure 1) for a range of droplet diameters as a function of water mist loading, assuming a monodisperse mist aerosol. The flame speed decreases sharply with increasing mist loading as the droplet diameter is decreased, indicating that the larger droplets are less efficient than smaller droplets in suppressing the flame because they may not evaporate completely prior to entering the flame zone.

---

[*] For further background and publications on the water mist project, see the Center for Commercial Applications of Combustion in Space (CCACS) webpage: http://www.mines.edu/research/ccacs/Fire_Suppression/Mist.html.

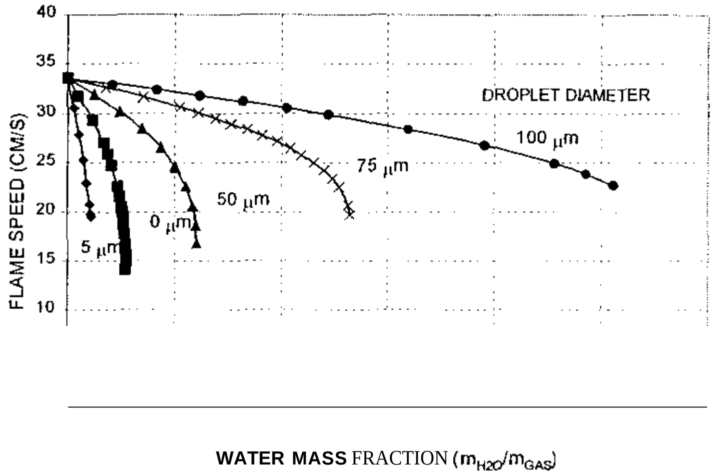

Figure 1. The effect of droplet diameter and water mass fraction on the propagation speed of a CH_4-air flame.

An examination of the relative effects of sensible and latent heats on flame-propagation speed shows that the predominant effect is due to sensible, rather than latent heat for the conditions modeled. Using non-physical computer inputs for the model allows these effects to be decoupled so that the relative magnitude of the individual effects can be studied. Figure **2** shows the sensible and latent heat effects as a function of water mist loading for *50* μm diameter droplets on a CH_4-air flame.

Investigation into the effect of absorption of radiation by the water-mist droplets shows a slight inhibiting effect of flame propagation speed. This effect is primarily due to an increase in the evaporation rate of the droplets prior to encountering the flame. A more complete examination of this fire-suppression mechanism is reported in [8].

WATER MIST AEROSOL DYNAMICS

The primary goal of this model is to better understand the character of the water mist as it exists in the flame tube prior to encountering the flame front. A model is being developed that combines computational fluid dynamics using the CFD-ACE+™ [9] software with aerosol characterization using the MAEROS software [10]. The information provided by this model is initially intended to provide size distribution and droplet concentration input for the fire suppression model as applied to the experiments previously described. In these experiments, the mist is allowed a one-minute relaxation time during which it decelerates, coagulates, and deposits on the tube **walls.** In the future this model will be adapted to suit the more complex experimental conditions inherent in normal gravity and in difficult geometries.

The modeling approach begins with creating a block centered mesh of the experimental system. CFD-ACE+™ is then used to compute a velocity vector, v(r,z), for the mist droplets in each of the cells during each time increment. **As** written, the MAEROS software assumes a stagnant, spatially homogeneous mist, however, it is possible to modify the general dynamic equation for aerosol evolution to include only the coagulation mechanisms that apply to a given set of conditions. In this case, a laminar shear coagulation kernel describes the experimental conditions [11],

$$K(a,b) = \frac{4}{3}G(a+b)^3 \qquad (1)$$

where G is the scalar magnitude derived from the velocity gradient tensor between droplets of radii ***a*** and ***b*** in adjacent cells.

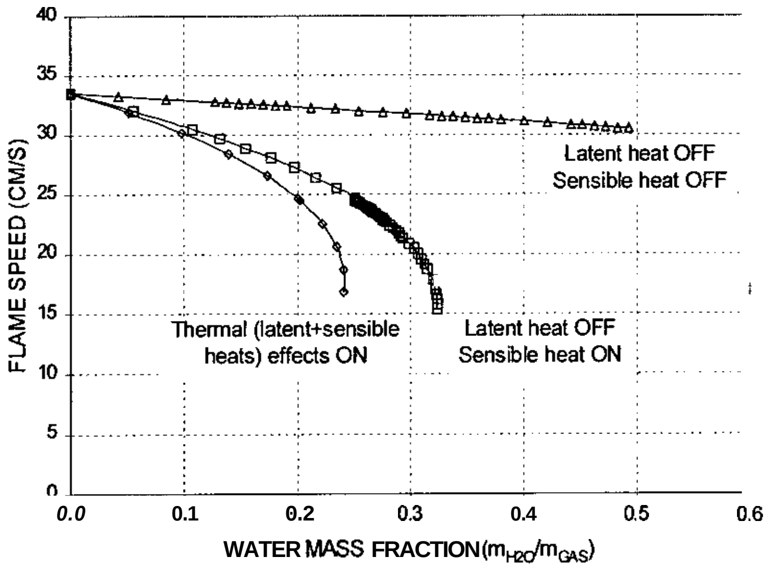

Figure 2. Effect of water mass fraction and sensible and latent heats on the propagation speed of a CH_4-air flame in a 50-µm droplet water mist.

Given velocity-gradient scalar values calculated using the vectors generated by CFD-ACE+™, MAEROS computes droplet size distribution and number density of the mist droplets in each of the blocks during a time increment. A particle-tracking algorithm borrowed from contaminant transport modeling [12] is employed to identify droplets as they travel from block to block. This information is used as input for MAEROS as the initial aerosol concentration for the block. MAEROS also allows a source term for blocks that are adjacent to a mist nozzle. The droplets that arrive at the outermost layer of blocks are counted as having been deposited on the surface and are removed from the aerosol with 100% efficiency. This deposition algorithm replaces the existing deposition kernels in the MAEROS software. A flowchart of the overall modeling approach is given in Figure 3.

CONCLUSIONS AND FUTURE WORK

CONCLUSIONS

With respect to the modeling of fire-suppression mechanisms at the interface of water mists and CH_4-air flames, the flame propagation speed decreases sharply with increasing mist loading as droplet diameter is decreased. This indicates that the larger droplets are less efficient in suppressing the flame because they do not completely evaporate prior to encountering the flame. The relative effects of sensible and latent heats on flame propagation speed show that the predominant effect is due to sensible, rather than latent heat due to the high temperature of the flame. Preliminary investigation into the effect of absorption of radiation by the water mist droplets shows a slight inhibiting effect of flame propagation speed, an effect is primarily due to an increase in the evaporation rate of the droplets prior to encountering the flame.

A model that combines computational fluid dynamics with aerosol characterization is being developed. The information provided by this model will initially be used to determine the wall deposition rate and to track the movement and changes in size distribution and droplet concentration of the mist aerosol from the time it is injected into the flame tube until it encounters the flame. Eventually this model will be adapted for use in normal gravity conditions to facilitate further experimentation.

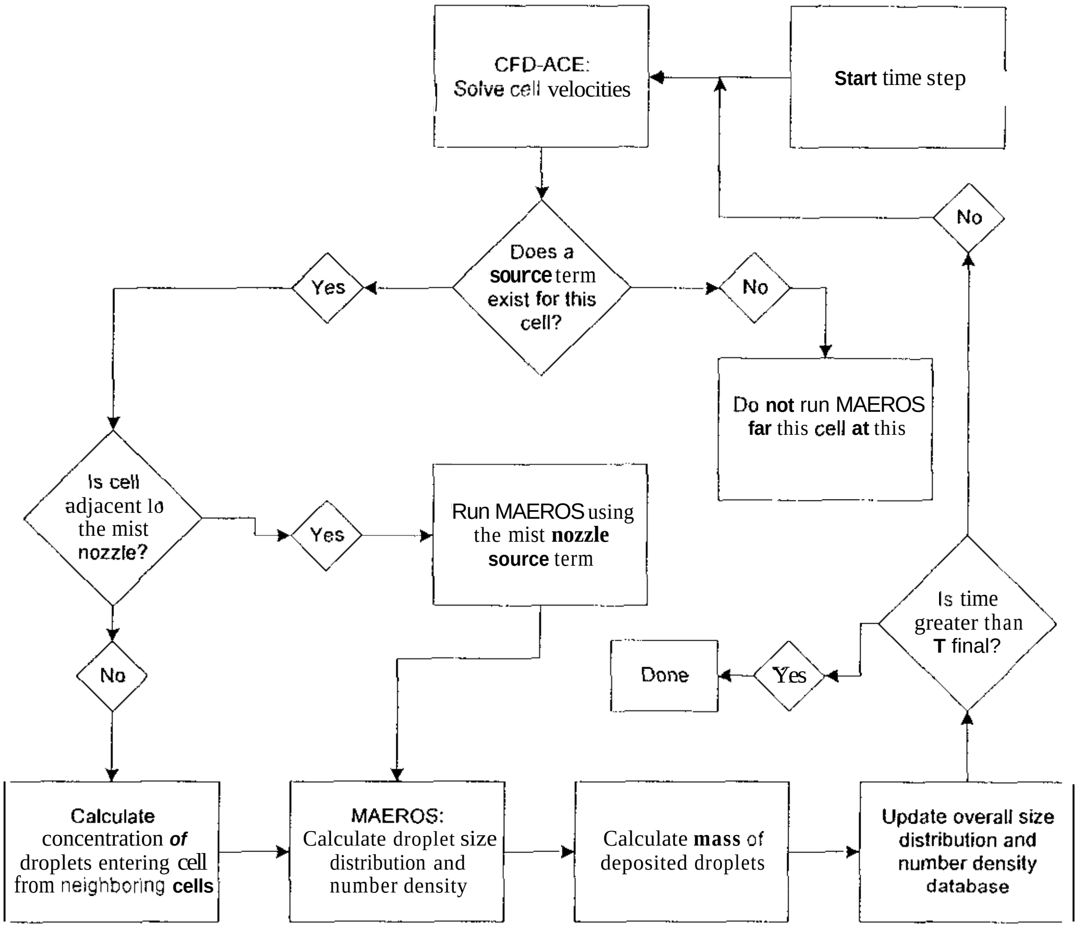

Figure 3. Flowchart of preliminary water-mist aerosol modeling approach

FUTURE WORK

In the modeling of the fire suppression mechanisms of fine water mist, the GRI-Mech reaction mechanism for methane combustion [13] was used in favor of a C_3H_8-air reaction mechanism because of its wide acceptance and ease of incorporation into the model. In the future, a C_3H_8-air reaction mechanism will replace the GRI-Mech mechanism to better simulate the experimental conditions. Work is currently being completed on the radiation absorption component of this model as well. The model will be calibrated and verified with experimental data available from the STS-107 flight.

When the aerosol model is functional, it will be calibrated and verified with experimental data obtained from KC-135 flights and from STS-107. It will then be upgraded as needed to apply to increasingly complex experimental conditions.

ACKNOWLEDGMENTS

This research is funded through the Center for Commercial Applications of Combustion in Space (CCACS) at the Colorado School of Mines (CSM). We wish to acknowledge the invaluable help of the CCACS director, Frank Schowengerdt and the guidance of Prof. J. P. Delplanque.

REFERENCES

1. Mawhinney, J. R., and Solomon, R. S., "Water Mist Fire Suppression Systems," Section 6, Chapter 15, *Fire Protection Handbook,* 18th Edition, National Fire Protection Association, Quincy, MA, 1997.
2. Wolfe, J., Brooks, J., and Walker, J., *Full-Scale Aircraft Cabin Twin Fluid, Low Pressure Water Mist Fire Suppression System Proofof-Concept Evaluation,* Draft Technical Report, Naval Air Systems Command, 2000.
3. Prasad, K., Patnaik, G., and Kailsanath, K., *Advanced Simulation Toolfor Improved Damage Assessment 2) Water-Mist Suppression of Large Scale Compartment Fires,* Report NRL/MR/6410—00-8507, Naval Research Laboratory, 2000.
4. Abbud-Madrid, A., Riedel, E. P., and McKinnon, J. T., "Effects of Water Mists on Premixed Flame Propagation in a Buoyancy-Free Environment," *Preceedings,* Halon Options Technical Working Conference, Albuquerque, NM, pp. 295-300, 1999.
5. Yang, W., and Kee, R. J., "A Modeling Study of the Effects of Water Mists on Premixed Methane-Air Flames," *Proceedings,* Western States Section Combustion Institute, Spring Meeting, Paper Number SOO-0054, March 2000.
6. Kee, R. J., Grcar, J. F., Miller, A., and Meeks, E., *Premix: A Fortran Programfor Modeling Steady Laminar One-Dimensional Premixed Flames,* Technical Report, Sandia National Laboratories, 1998.
7. Kee, R. J., Rupley, F. M., Meeks, E., and Miller, J. A., *CHEMKIN-III: A Fortran Chemical Kinetics Packagefor the Analysis of Gas-Phase Chemical and Plasma Kinetics,* Technical Report SANDSO-8003, Sandia National Laboratories, Livermore, CA, 1980.
8. Yang, W., Parker, T., Kee, R. J., McKinnon, J. T., and Abbud-Madrid, A., "The Influence of Water-Mist and Thermal-Radiation Interactions on the Structure and Extinction of Premixed Methane-Air Flames," Paper No. 19, *Proceedings,* Second Joint Meeting of the US Sections **of** the Combustion Institute, Oakland, CA, March 26-28,2001,
9. CFD Research Corp., "CFD-ACE+ Version 6," **http://www.cfdrc.comldatab/sofhvare/aceplud,** Huntsville, AL, 1999.
10. Gelbard, F., "MAEROS Multicomponent Aerosol Time Evolution," *Radiation Safety Information Computational Center Code Package PSR-466,* Oak Ridge National Laboratories, TN, 2000.
11. Williams, M. M. R., and Loyalka, S. K., *Aerosol Science Theory and Practice,* Pergamon Press, Oxford, England, pp. 170-172, 1991.
12. Zheng, C., and Bennet, G. D., *Applied Contaminant Transport Modeling,* John Wiley and Sons, Inc., NY, pp. 105-150, 1995.
13. Bowman, C. T., Hanson, R. K., Gardiner Jr., W. C., Lissianski, V., Frenklach, M., Goldenberg, M., and Smith, G. P., *GRI-Mech* – An *Optimized Detailed Chemical Reaction Mechanismfor Methane Combustion and NOformation and Reburning,* Report 97-0020, Gas Research Institute, 1997.