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COMPUTER SIMULATION OF THE LIQUID AGENT SPRAY MOTION AND EVAPORATION

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ABSTRACT

The discharge of a liquid fire extinguishing agent stored in a pressurized vessel through an orifice generates a freely moving spray outside the vessel. The flow has been modeled as a two-phase, three-component, turbulent, compressible, dissipative flow. It has been assumed that the gaseous phase consists of agent vapor, nitrogen and oxygen, whereas the liquid consists of agent only. Viscosity, heat conduction, mass diffusion and turbulence have been included in the description. Interphase processes; such as Stokes forces and aerodynamic drag, forced convection and evaporation; have also been included. The spray is assumed to be a monodispersed phase described by the Sauter mean diameter. All the transport coefficients, the specific heats and the vapor pressure equation are temperature dependant. The impact of the gravitational field on the momentum exchange has also been included. The mathematical model describing the physical phenomena has been formulated with the use of the partial differential equations associated with the relevant initial-boundary conditions, expressing the balances of mass, momentum and energy. The set of time-dependant equations has been referred to the two-dimensional cylindrical geometry. The equations have been solved numerically with the use of time-marching finite-difference partially implicit scheme. The Conchas-Spray computer code of Los Alamos National Laboratory has been used to run the calculations. Sample results obtained for an extinguishing agent have been presented and the potential of the model and computer code have been discussed.

INTRODUCTION

The work is part of a comprehensive research program carried out at the National Institute of Standards and Technology, focusing on identifying alternatives to halon 1301 for in-flight aircraft fire protection. The alternatives should be effective fire extinguishing agents and should not create unacceptable safety, environmental and systems compatibility problems. The fundamental CFD problem for an extinguishing agent discharge and dispersion is to develop the capability of qualitatively and quantitatively predicting the time evolution of the agent concentration field. It inherently involves a multidimensional analysis of a one- or two-phase, multi-component, compressible medium where thermodynamic effects and transport phenomena are important. The dispersion of sprays of halon and halon-alternative fire extinguishing agents throughout a protected space is a very complex process involving many physical phenomena occurring simultaneously and affecting each other. The agent stored in the liquid state is discharged from nitrogen-pressurized vessels through a simple, nozzle/orifice-like exit [1]. The systems under consideration involved vessel volumes of the order of $10^{-3}/m^3$, with required discharge times of the order of $10^{-2}/s$. To achieve such rapid discharge times, the pre-pressurization levels must typically be of the order of thousands of kilopascals. As the agent exits from the vessel, thermodynamic and fluid-dynamic instabilities lead to flashing and break-up of the agent into a two-phase droplet/gaseous jet mixture. This occurs in a relatively short transition region which starts at the vessel exit and ends at a section of the two-phase jet where thermodynamic and fluid-dynamic instabilities have ceased. Downstream of this "initial section" [2], the flow begins to develop as a mixed, two-phase, agent/air jet where thermodynamic equilibrium is assumed to be maintained and where droplet collision and agglomeration do not play an important role in the ensuing jet dynamics and in the dispersal of the agent throughout the protected space. At the initial section

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the spray consists of a mixture of liquid-agent fragments of various shapes and sizes and gaseous agent. This then entrains initially quiescent air from the surrounding outside environment. Because the temperature of the discharged liquid agent is far above its atmospheric-pressure boiling point, it very quickly evaporates and creates a cloud of agent vapor surrounding the moving spray. The entrainment, mixing and evaporation continue as the spray is dispersed throughout the space.

MATHEMATICAL MODEL

The mathematical model used in the calculations is in general consistent with the equations included in the Conchas-Spray computer code [3] designed for the spray systems. The process has been described from the fundamental point of view as a two-phase, three component, turbulent, compressible, dissipative flow. It has been assumed that the gaseous phase consists of the following three components: agent vapor, nitrogen and oxygen, whereas the liquid phase consists of the liquid agent only. Within the gaseous phase, heat conduction, mass diffusion, and the viscosity have been taken into account as well as the impact of turbulence affecting the dissipation and mixing. Also taken into account are interphase processes such as momentum exchange in the form of Stokes forces and aerodynamic drag between the droplets and the gaseous phase, heat exchange in the form of forced convection, and mass exchange in the form of evaporation. It has been assumed that the spray droplets are described by Sauter mean diameter. The evaporation process has been expressed in terms of a quasi-steady model. The impact of turbulence on the droplet motion within the spray has also been taken into account. The turbulence in the gaseous phase has been described with the use of the Deardorff model [4], relating the velocity gradients to the turbulent viscosity. The transport coefficients, heat conductivity, mass diffusivity, and viscosity, as well as the specific heats are temperature dependent. The vapor pressure equation is a strongly non-linear function of temperature and the dependence is approximately exponential. The impact of the gravitational field as an external volume force has also been included. It has been assumed that no chemical reactions and associated effects (like heat release) occur in the system. The governing equations express the balances of mass, momentum and energy for the medium under investigation. This is an initial/boundary value problem within a region bounded by the initial section and the far-field boundaries of the protected space. The set of time-dependent equations was expressed in a two-dimensional form since the experimental discharges were designed to be axisymmetric. The total mass density of the fluid (excluding the mass of the spray droplets) is defined in terms of a partial mass density of the component species. The mass balance equates the change in species concentration with time to the sum of the advection, diffusion and source terms due to evaporation of that particular component. The total fluid density satisfies the total mass balance equation, recognizing that the net diffusion must sum to zero. The momentum balance equations in the axial and radial directions for the fluid mixture set the time rate of change of momentum equal to the sum of the advection, pressure, viscous stress, droplet drag, and body force terms. The energy equation for the gas phase accounts for the local change in specific internal energy from the sum of the net advection of sensible heat, heat conduction, enthalpy transport accompanying the diffusion of individual species, flow work, viscous heating, and energy transfer between the two phases. The state relations are assumed to be those of an ideal gas mixture. The transport coefficients include the laminar and turbulent contributions to the momentum, heat and mass transfer. The turbulent viscosity is broken into a constant uniform background term and a variable turbulent viscosity. The thermal and mass turbulent diffusivity are related to the viscosity through the local Prandtl and Schmidt numbers of the gaseous mixture. The motion of the droplets in the spray is governed by ordinary differential equations in Lagrangian form. It has been assumed that the spray is sufficiently thin, and, as a consequence, the volume displaced by the droplets may be neglected. Velocity components in the axial, radial and swirl directions are tracked and the transport between phases is dependent upon the Reynolds number computed from the slip velocity and the film temperature and composition. Internal droplet motion is ignored, leading to a particle uniform in temperature. The mass of the droplets change in time due to evaporation according to the model of Dukowicz [5]. The particle velocity is computed from the drag associated with the slip velocity. The latent heat cools the droplet during evaporation, and the heat transfer between the drop and the environment is

determined using the Ranz-Marshall correlation [6], modified to account for mass leaving the surface [7]. The fluid-particle interactions are all two-way coupled to ensure overall conservation of mass, momemtum and energy.

COMPUTATION RESULTS

All the computations with Conchas-Spray have been performed on a Convex supercomputer with a Unix operating system. The results have been presented graphically as contours of constant velocity, density, pressure, temperature, species concentration, vorticity, kinematic viscosity, mass flux, and liquid phase. The configuration investigated was the discharge of a droplet spray with properties similar to one of the agents into a totally closed enclosure. The nozzle was located on the centerline of the 0.42 m diameter cylindrically shaped volume. Agent inflow boundary conditions, including temperature, density, and velocity were estimated from the results of the discharge vessel experiments [1] and specified in the calculation. Also, it was assumed that the spray is already established at the discharge orifice exit (at zero-length transition region) where it is injected into the enclosure in the liquid phase at the specified rate. In this regard, the reader is referred to Cooper [2] who develops and applies a model which predicts time-dependent vessel discharge and initial-section flow properties, including temperature, velocity, mass flux, and quality, but not droplet size distribution. Calculations reported here do not yet incorporate these latter results. The initial pressure was 101 kPa, and it was assumed that the liquid agent was initially delivered at this same pressure and at the normal boiling point temperature (-41°C). Computational parcels representing the droplets are introduced at the injector with an axial velocity of 61.4 m/s directed at an angle of 0° relative to the symmetry axis. A zero azimuthal component of velocity is assumed for the droplets at the injector. All the gas and liquid parameters have been assumed to be uniform across the orifice exit. All the parameters within the compartment have been assumed to be uniform as well at zero time. The compartment surrounding walls have been treated as solid boundaries maintained at a constant temperature of 21°C. Free-slip boundary conditions have been assumed on the walls. Thus the subsequent penetration and shape of the spray result solely from the interactions of the liquid droplets with the ambient air. The numerical solution of the balance equations associated with the initial and boundary conditions and the material properties provides the time evolution of the spray in the space. One should emphasize that realistic results from Conchas-Spray-like modeling of the spray dispersion process would appear to be dependent on the validity of the transition-region concept and on the ability to provide reasonable estimates of the state of the spray at the initial section, i.e., the boundary conditions. In this regard, it is beyond the state of the technology to be able to model accurately the details of the disc rupture or its impact on the agent dispersion problem. Also, in spite of the fact that initial-section droplet size distribution may play an important role in agent dispersal, a method of estimating this does not seem to be forthcoming soon (as mentioned, it is not included in the model of Cooper [2]. In the present calculations the droplet size distribution could only be hypothesized.

Figure 1 to Figure 4 illustrate (discharge downward - figures rotated by 90°) the vapor density, temperature, pressure and gaseous phase overall density contour field time development of the agent spray under the following conditions: initial droplet diameter of 200 μm, enclosure length of 1 m, and initial ambient temperature equal to the 21°C. The distribution of agent concentration versus time is an important piece of information for the determination of active inhibiting areas interacting with a flame. One can see in Figure 1 that the spray develops essentially in the form of a cone with a fat head growing in time. Thus, most of the active inhibiting area is located downstream, at a distance from the discharge orifice. A vortex which tends to develop within the head of the spray enhances the process of formation of the suppression zone. Figure 2 shows the distribution of the gaseous phase temperature within the spray. An interesting effect is the generation of temperatures locally which exceed the initial temperature. It turns out that the maximum gaseous phase temperature is higher by 41° relative to the initial ambient temperature. The phenomenon can be explained in terms of pressure waves, another interesting effect appearing due to medium compressibility created during the discharge process, which compress the gas. The vaporization of the agent cools the chamber, but locally it is possible to have the temperature increase by compression

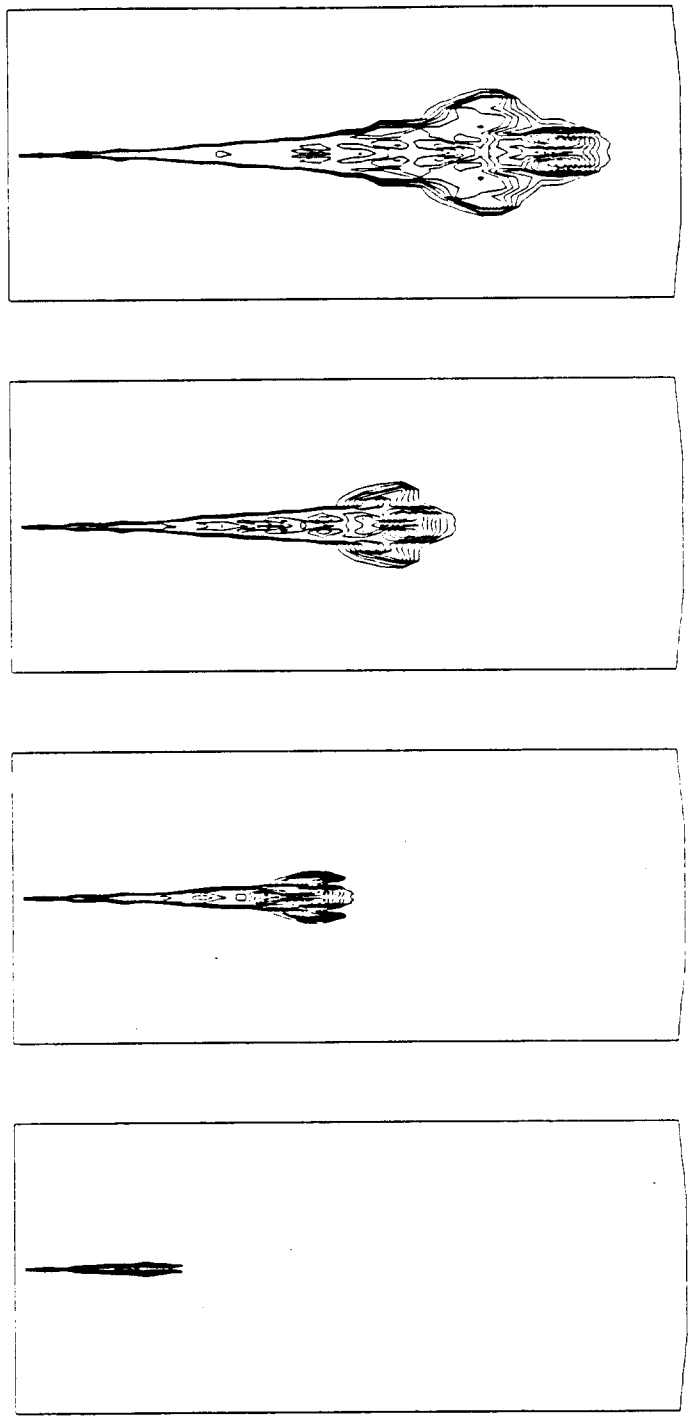

Fig.1 Vapor density maps at: 3.5, 8.3, 10.7, 14.3 ms (upward) - the outline value 0.032 kg/m^3. Initial spray angle 0°. Spray mean diameter 200 μm. Ambient T = 294 K and P = 101 kPa. Compartment 1 x 0.42 m.

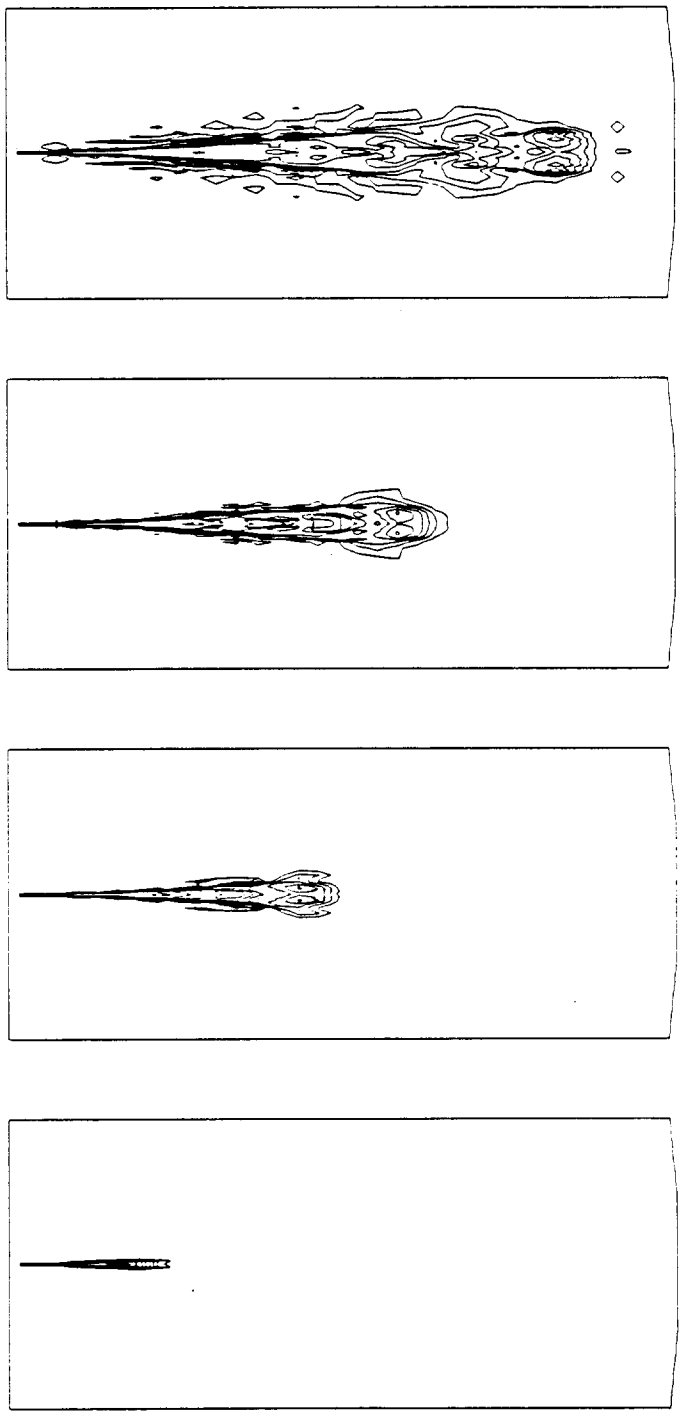

Fig.2 Gas phase temperature maps at: 3.5, 8.3, 10.7, 14.3 ms (upward) - the maximum value 335 K. Initial spray angle 0°. Spray mean diameter 200 μm. Ambient T = 294 K and P = 101 kPa. Compartment 1 x 0.42 m.

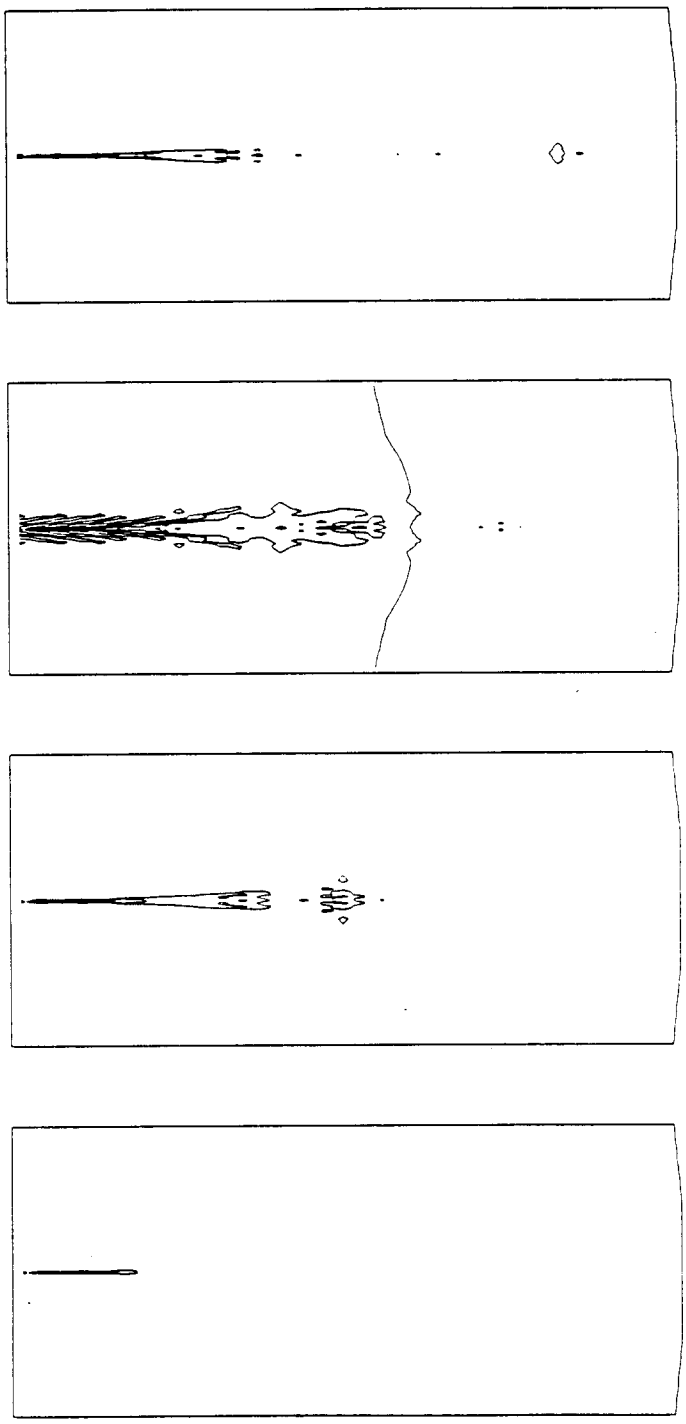

Fig.3 Gas phase pressure maps at: 3.5, 8.3, 10.7, 14.3 ms (upward) - the outline value 105 kPa. Initial spray angle 0°. Spray mean diameter 200 μm. Ambient T = 294 K and P = 101 kPa. Compartment 1 x 0.42 m.

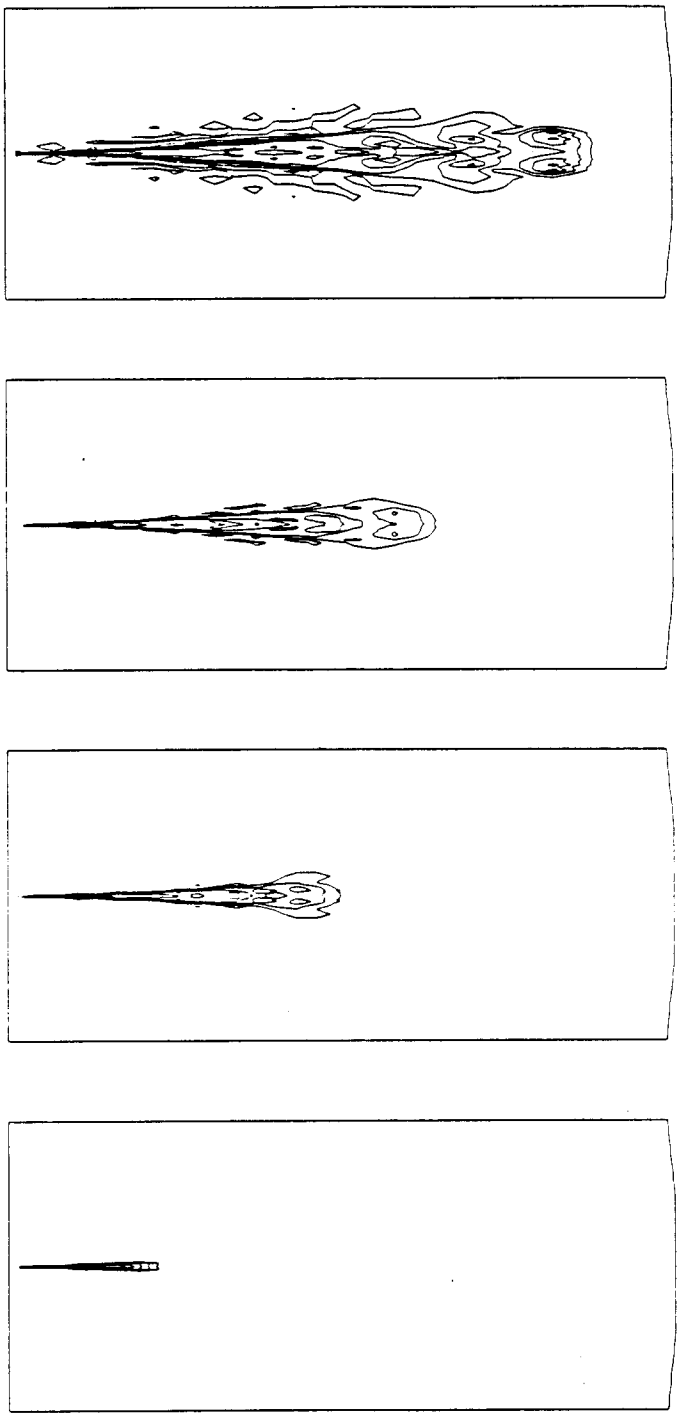

Fig.4 Gas phase density maps at: 3.5, 8.3, 10.7, 14.3 ms (upward) - the outline value 1.27 kg/m^3. Initial spray angle 0°. Spray mean diameter 200 μm. Ambient T = 294 K and P = 101 kPa. Compartment 1 x 0.42 m.

which outweighs the temperature decrease due to vaporization. That in turn influences the interphase heat exchange rate which depends on the surface area and temperature difference. An example of a pressure wave occuring in the spray flow field is shown in Figure 3 (particularly well seen on the third picture at 10.7 ms). Locally, where the temperature of the gas phase becomes close to the agent boiling point, the Mach number may exceed the sonic condition (the speed of sound decreases with the square root of absolute temperature), which means that a shock wave is created. The wave appears soon after the begining of the discharge process and travels supersonically toward the bottom wall. After reflection it travels upward encountering the spray moving in the opposite direction. Due to a significant difference in the velocities, a momentum exchange between the spray and pressure wave occurs. That influences the spray shape, velocity and penetration. This interaction is one of the causes of the spray fat head. Such a phenomenon may be of importance when an agent is discharged in very small compartments or in areas of a complex geometry. Figure 4 shows the distribution of the overall gaseous phase density within and around the spray. The contours look a little broader than the agent vapor isolines and that results from the fact that some amount of the air is entrained into the spray from the surroundings. The air mixes simultaneously with the agent vapor and liquid droplets. The pictures provide the information necessary for the analysis of the dynamics of the agent spray motion and evaporation. Eventually, it gives an engineering input for the designers of the agent delivery systems.

CONCLUSIONS

1. The CFD model and computer code can be used effectively to analyze the dynamics of halon-alternative agent dispersion and mixing in a space designed for fire protection. Within its physical limitations, it can perform the necessary computations of the discharge process quickly and relatively cheaply, aiding one's understanding and indicating directions for experiments and design work.
2. The numerical analysis based on the full fluid dynamics equations as well as a description of the heat and mass transfer leads to the time dependance of the two-dimensional field of all parameters characterizing the agent dispersion phenomena, including species concentration, pressure, temperature, velocity, spray contour and penetration. Much of these data are difficult or impossible to measure in experiments.

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