Development and evaluation of two new droplet evaporation schemes for fire dynamics simulations

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ARTICLE INFO

ABSTRACT

The evaporation of sprinkler droplets is an important phenomenon in fire simulations both for heat removal from the gas and for heat removal from surfaces. In this paper, we address the problems of potential numerical instability and super-saturation that may occur in explicit time integration of the droplet equations. Two novel numerical approaches are developed and evaluated. The first is based on an analytical solution that relaxes the cell composition and temperature toward the equilibrium values. The second method is an implicit solution to the droplet equations. The two approaches are implemented in the Fire Dynamics Simulator (FDS) and verified and validated using both single droplet and practical sprinkler calculations. Ultimately, the implicit approach is deemed the most cost effective for practical fire simulations.

1. Introduction

The evaporation of sprinkler droplets is an important phenomenon to consider when modeling the thermal environment due to a fire. For standard large drop sprinklers (not a watermist system), efficacy of droplets have been estimated analytically [1] and confirmed experimentally [2] to remove between 11% and 26% of the heat produced by a fire. Watermist systems can remove 100% of the heat produced by a fire either by extinguishment or by providing sufficient evaporation to maintain compartment temperatures at or below the boiling point of water [3]. Capturing the dynamics of these systems in design or forensic applications requires an accurate and robust droplet evaporation model, which is the topic of the present paper.

A successful model of droplet evaporation in fire dynamics simulations should

(1) accurately represent droplet dynamics
(2) conserve mass and energy
(3) be computationally efficient
(4) be numerically stable
(5) obtain the correct equilibrium state
(6) be independent of the order in which the droplets are processed

Typical computational fluid dynamics (CFD) codes use either stiff explicit or segregated implicit ODE time integrators to solve the droplet dynamics equations (see, e.g., [4]). These solvers, in general, satisfac-torily address the issues of accuracy and conservation (Items 1 and 2), and stability (Item 4). However, stability often comes at the expense of efficiency (Item 3), which is of particular concern for practical applications in fire modeling.

To address computational efficiency (Item 3) CFD codes do not track every droplet from a sprinkler—the computational cost would be too high. Instead, a smaller number of "superdroplets" are tracked, where each superdroplet represents many individual real droplets with the same diameter and thermophysical properties. This approach, while cost effective, can lead to extremely high rates of heat and mass transfer when very fine droplets require a large superdroplet weighting factor. These high heat and mass transfer rates present significant numerical challenges for computational efficiency and numerical stability (Item 4). The methods presented in this paper are aimed at addressing these two critical, practical issues in droplet evaporation for fire modeling applications.

The methods discussed in this work also address equilibrium (Item 5) and droplet processing order (Item 6). These are subtle issues that are discussed in more detail later in the paper.

The NIST Fire Dynamics Simulator (FDS) [5,6] has seen a number of approaches to droplet evaporation in an attempt to achieve the desirable model attributes listed above. A brief history is summarized below:

FDS 1−4 used an explicit solver for the heating and evaporation of droplets. During this time period, development of routines for droplet transport and evaporation focused on applications like the sprinkler

Nomenclature

Nomenclature

A	surface area (m^2), computational time (s)
B, C	computational time per droplet (s/droplet)
c	heat capacity (J/kg/K)
F, G	droplet temperature solution components
H	enthalpy (J)
h	heat transfer coefficient (W/m^2/K)
h_l	liquid enthalpy (J/kg)
h_m	mass transfer coefficient (m/s)
h_v	heat of vaporization (J/kg)
M	total normalized vaporization rate (1/s)
N	number of particles per cell
m	droplet mass (kg)
$\dot{q}_r$	droplet radiation absorption (W)
t	time (s)
T	droplet temperature (K)
T_g	gas temperature (K)
T_w	wall temperature (K)
Y	vapor mass fraction (kg/kg)
V	cell volume (m^3)

Greek

β	analytical solution parameter (kg$^{1/3}$/s)
$\hat{\delta t}$	small time step (s)
Δt	time step size (s)
ρ	gas density (kg/m^3)
χ	area per mass factor (m^2/kg$^{2/3}$)
ω	relaxation time constant (1/s)

superscripts

n	time step

subscripts

eq	cell equilibrium condition
f	film
g	gas
i	droplet index
l	liquid at equilibrium
m	mass transfer
v	vapor, vaporization
w	wall

suppression of a commodity using a simple exponential decay of the heat release rate based on the delivered quantity of water [7].

FDS 5 came with a significant overhaul to the droplet model. This in large part resulted from efforts to model water mist systems where the approach taken in FDS 1−4 resulted in numerical instabilities. In a water mist system, especially upon initial discharge, very large changes in droplet temperature and gas temperature can occur. The explicit approach being used could result in large, non-physical swings in gas and droplet temperature leading to numerical instabilities. The droplet model was changed to a semi-implicit method where the droplet mass and temperature were solved implicitly and the gas temperature (and wall temperature for a droplet on a solid surface) was solved explicitly. This approach resolved many of the issues with numerical instabilities. As more rigorous verification and validation practices were employed in FDS development, this semi-implicit approach underwent further modifications to ensure the conservation of energy.

FDS 6 introduced some additional changes to the droplet model. Most notably, a self-consistent set of thermophysical properties was introduced for common species using NIST-JANAF data [8]. This effort ensured the correct equilibrium state was being reached. Users of FDS continued trying to expand its application space with applications including very fine watermist (fog) and sprinkler suppression of pyrolyzing materials. The FDS 6 routine had difficulties with these two classes of problems: droplets impacting hot surfaces with low conductivity and low thermal inertia (for example foams) and simulations with very fine watermist. The root cause in both cases was that the explicit solver being used for the gas and wall temperatures was resulting in large overshoots or undershoots in temperature prediction. This resulted in anomalous temperatures in the simulation or runtime failures when erroneous temperature values were used in other subroutines.

2. Development of new evaporation schemes

While many existing CFD models have successful droplet evaporation algorithms, these algorithms generally do not satisfy computational efficiency requirements for FDS. In this work, two new schemes are developed and evaluated to address the shortcomings of the other methods discussed above. The first is a relaxation method based on an analytical solution to an alternate set of droplet equations. The second

is an implicit, drop-wise approach (which we ultimately determine to be superior in terms of computational cost and ease of implementation). Both of these approaches are novel methods of solving the droplet equations.

Below we present the governing equations followed by an overview of the new schemes. Details are provided in Appendices A and B.

3. Governing equations

The governing equations for droplet evaporation are given below and may be found in Ref. [9]. Summations are over all droplets in a computational cell. Again, note that each individual droplet represents a superdroplet with a mass weighting factor (omitted here to avoid complicating the equations). Details may be found in [5].

$$\frac{\mathrm{d}m_i}{\mathrm{d}t} = A_i h_{m,i} \rho (Y_v - Y_{l,i}) \tag{1}$$

$$\rho V \frac{\mathrm{d}Y_v}{\mathrm{d}t} = -\sum_i \frac{\mathrm{d}m_i}{\mathrm{d}t} \tag{2}$$

$$m_i c_i \frac{\mathrm{d}T_i}{\mathrm{d}t} = A_g h_g (T_g - T_i) + A_w h_w (T_w - T_i) + \frac{\mathrm{d}m_i}{\mathrm{d}t} h_v + \dot{q}_r \tag{3}$$

$$m_g c_g \frac{\mathrm{d}T_g}{\mathrm{d}t} = -\sum_i \left(A_g h_g (T_g - T_i) + \frac{\mathrm{d}m_i}{\mathrm{d}t} (h_v + h_l) \right) \tag{4}$$

$$m_w c_w \frac{\mathrm{d}T_w}{\mathrm{d}t} = -\sum_i A_w h_w (T_w - T_i) \tag{5}$$

Eq. (1) defines the droplet evaporation as a function of the droplet surface area, A_i and a mass transfer coefficient, $h_{m,i}$, times the difference in the gas vapor fraction, Y_v, and the droplet surface vapor fraction, $Y_{l,i}$, evaluated using the Clausius-Clapeyron equation. Note that condensation is not presently modeled in FDS.

Eq. (2) defines the rate of change in vapor mass in a gas cell as the sum of the evaporation rates of the droplets in the cell. Note that for the purposes of this paper we are discussing the change of water vapor concentration due to evaporation only. Water created via combustion is handled in a separate routine, which is time split from the evaporation routine.

Eq. (3) defines the rate of change in the droplet temperature, T_i.