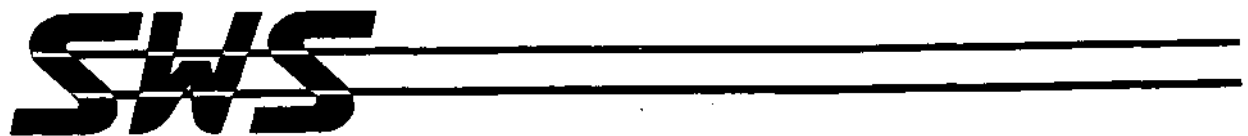# A One-dimensional Numerical Model
for the Computation of the Transient Temperature
of Liquid and Solid Drops in Free-fall

by K. C. Tang and Robert R. Czys

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Atmospheric Sciences Division
Illinois State Water Survey
Champaign, Illinois

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Abstract

This document describes a one-dimensional heat and mass transfer numerical model that was developed to study the temperature and freezing of raindrops in free-fall. The numerical model included the effects of ventilation and mass transfer on the disposal of heat, as well as the effects of mass transfer on drop size and drop fall speed. For liquid raindrops, the temperature distribution inside the drop is simulated by considering the heat conduction problem within the liquid drop. A modified version of the one-dimensional model is also presented to simulate raindrop freezing.

Nomenclature

List of Symbols

c_p	specific heat capacity
d	drop diameter
D	diffusivity
f_v	ventilation factor defined by Eq. (18)
h	heat transfer coefficient or enthalpy
h_{sf}	latent heat of melting
h_{sg}	latent heat of sublimation
m	mass fraction
m	mass flow rate
m''	mass flux
N_{Pr}	Prandtl number
Nu	Nussult number
N_{Re}	Reynolds number
N_{Sc}	Schmidt number
q''	heat flux
r	spatial coordinate
R	drop radius
t	time coordinate
t^*	nondimensional time coordinate defined by Eq. (4)
T	temperature
T^*	nondimensional temperature defined by Eq. (3)
u	velocity
x	nondimensional spatial coordinate defined by Eq. (2)
$\mathbf{a}$	thermal diffusivity
	heat conductivity
v	kinematic viscosity
p	density

List of Subscripts

0	initial condition		v	vapor
$conv$	convection		w	water
mt	mass transfer by evaporation/condensation		$\propto$	environment condition
i	ice		o	outer edge
m	air-vapor mixture		s	drop surface
max	maximum		t	time coordinate
min	minimum			
$subl$	sublimation			

The Heat Conduction Problem

Following the discussion of Incropera and Dewitt (1985), the equation governing unsteady one-dimensional heat diffusion in a spherical coordinate system ($0 < r < R$) can be written in nondimensional form as:

$$\frac{\partial T_w^*(x,t^*)}{\partial t^*} = \frac{\partial^2 T_w^*(x,t^*)}{\partial x^2} + \frac{2}{x}\frac{\partial T_w^*(x,t^*)}{\partial x}, \tag{1}$$

with the nondimensional parameters defined as:

$$x = \frac{r}{R}, \tag{2}$$

$$T_w^*(r,t) = \frac{T_w(r,t) - T_{\infty,0}}{T_{\infty,min} - T_{\infty,0}}, \tag{3}$$

$$t^* = \frac{\alpha_w t}{R^2}, \tag{4}$$

$$\text{and } \alpha_w = \frac{\lambda_w}{\rho_w c_p}. \tag{5}$$

The left-hand side of Eq. (1) represents the rate of change of internal energy of the medium per unit volume. From conservation of energy, the left-hand side of the equation is equal to the net heat flux into the control volume.

Equation (1) presents a classic boundary value problem depending on the physical boundary conditions and initial time. For this problem, the conditions were:

$$\frac{\partial T_w^*(x=0,t^*)}{\partial x} = 0, \tag{6}$$

$$\text{and } \frac{\partial T_w^*(x=1,t^*)}{\partial x} = -\frac{R q_w''}{\lambda_w(T_{\infty,min} - T_{\infty,0})}, \tag{7}$$

where q_w'' is the heat flux conducted from the drop to the environment. Equation (6) is the symmetrical boundary condition, which states that initially there is no temperature gradient at the center of a water drop. Equation (7) is the boundary condition for a convective and evaporating surface at $r = R$. The heat flux conducted out of water drop q_w'', must be disposed of and carried away into the environment, and can be written as:

$$q_w'' = q_{conv}'' + q_{mt}'',\qquad(8)$$

where q_{conv}'' is the heat flux to be dissipated from the drop to the environment due to heat convection, and q_{mt}'' is the dissipated heat flux due to evaporation/condensation. The initial condition for the heat diffusion equation is:

$$T_w^*(x,t^* = 0) = \frac{T_{w,0} - T_{\infty,0}}{T_{\infty,\min} - T_{\infty,0}},\qquad(9)$$

which states that the initial drop temperature is uniform throughout the drop.

Convective Cooling

The convective heat flux q_{conv}'' from a water drop to the environment may be expressed by Newton's law of cooling as:

$$q_{conv}'' = h(T_w(r = R,t) - T_{\infty,t}),\qquad(10)$$

where h is the average convective heat transfer coefficient for the entire surface, $T_w(r = R,t)$ is the surface temperature of a water drop at time t, and $T_{\infty,t}$ is the environment temperature at time t. Thus, q_{conv}'' results from a temperature difference between the drop and the environment flow field. The average convective heat transfer coefficient can be expressed as:

$$h = \frac{\lambda_m Nu}{2R},$$ (11)

where λ_m is the thermal conductivity of the air-vapor mixture and Nu is the Nussult number.

The correlation of Ranz and Marshall (1952) has sometimes been used to obtain Nu for a freely falling liquid water drop. However, Beard and Pruppacher (1971) found that Ranz and Marshall's correlation overestimated the Nussult and/or Sherwood numbers, which might be due to their experimental setup which used a glass capillar to suspend the drops. Beard and Pruppacher (1971) obtained improved parameterization of Nu from laboratory experiments with freely suspended drops in a wind tunnel. Their experimental results for drop diameters in the range of 40 to 1200 µm showed that:

$$Nu = 2 \begin{cases} 1.00 + 0.108(N_{Re}^{1/2} N_{Pr}^{1/3})^2, (N_{Re}^{1/2} N_{Pr}^{1/3}) < 1.4 \\ 0.78 + 0.308(N_{Re}^{1/2} N_{Pr}^{1/3}), (N_{Re}^{1/2} N_{Pr}^{1/3}) \geq 1.4 \end{cases}.$$ (12)

This relationship was found to be in good agreement with the numerical results of Woo and Hamielec (1971). In addition, Pruppacher and Rasmussen (1979) investigated the evaporation rate of large water drops falling at terminal velocity in air. Their results showed that the applicable range of Eq. (12) can be extended to drop diameters up to 5000 µm.

Evaporative Cooling

Mass Transfer in a Quiescent Environment

Several assumptions were made in calculating the evaporative flux of water vapor from the stationary drop to the surroundings: 1) that a one-dimensional quasisteady system existed; 2) that the flux of water toward or away from the drop does not change the environment; and 3) that the drop surface reaches thermodynamic equilibrium. Hence, following the discussion of Kays and

Crawford (1980) the water vapor species equation for a two-component mixture of water vapor and air (for $R < r < \infty$) using a one-dimensional spherical coordinate system can be written as:

$$\rho_m u_m \frac{dm_v}{dr} - \frac{1}{r^2} \frac{d}{dr}\left(r^2 \rho_m D \frac{dm_v}{dr}\right) = 0,$$

(13)

where m_v is the mass fraction of water vapor, ρ_m is the density of the mixture, u_m is the bulk velocity of the mixture, and D is the diffusivity of water vapor in air. The boundary conditions for the water vapor species equation were:

$$m_v(r = R) = m_{v,s},$$

(14)

$$\text{and } m_v(r \to \infty) = m_{v,\infty},$$

(15)

where $m_{v,s}$ is the mass fraction of vapor at the water drop surface, and $m_{v,\infty}$ is the mass fraction of vapor at the environment. By considering mass conservation at the water drop surface and the solution of the species equation (Eq. 13), the evaporation rate of mass flux from the water drop surface to the sounding can be written as:

$$\dot{m}_{mt,0} = 4\pi \rho_m D R \ln\left(\frac{1 - m_{v,\infty}}{1 - m_{v,s}}\right).$$

(16)

Finally, the heat flux from a stationary water drop to the water-air interface that provided the energy required to evaporate the water can be written as:

$$q''_{mt,0} = \dot{m}''_{mt,0}(h_w - h_m),$$

(17)

where h_w is the enthalpy of the liquid water, and h_m is the enthalpy of the vapor-air mixture at the drop surface.

Mass Transfer in a Convective Environment

The effect of convection on the mass transfer from a water drop to the surroundings due to the drop's motion was approximated by means of a ventilation coefficient, f_v, defined by:

$$f_v = \frac{m_{mt}}{\dot{m}_{mt,0}},$$ (18)

where m_{mt} is the evaporation rate of a moving drop, and $m_{mt,0}$ is the evaporation rate of a stationary drop. Relationships for f_v have been found experimentally for water drops evaporating in air during free-fall (Beard and Pruppacher 1971; Pruppacher and Rasmussen 1979):

$$f_v = \begin{cases} 1.00 + 0.108(N_{Sc}^{1/3} N_{Re}^{1/2})^2, & (N_{Sc}^{1/3} N_{Re}^{1/2}) < 1.4 \\ 0.78 + 0.308(N_{Sc}^{1/3} N_{Re}^{1/2}), & (N_{Sc}^{1/3} N_{Re}^{1/2}) \geq 1.4 \end{cases},$$ (19)

where $N_{Sc} = v/D$ is the Schmidt number given as the ratio of the kinematic viscosity v to the diffusivity D of water vapor in air. With the ventilation factor f_v, the latent heat required to evaporate the liquid water q_{mt}'' was obtained from:

$$q_{mt}'' = f_v \, \dot{m}_{mt,0}'' (h_w - h_m) = f_v \, q_{mt,0}''.$$ (20)

Simulation of Drop Freezing

When ice nucleates within a supercooled drop, complete solidification occurs in two major stages (see for example, Pruppacher and Klett, 1980; Dye and Hobbs, 1968). In the first stage, a small fraction of liquid water is frozen and releases latent heat, which almost immediately raises the temperature of the whole drop to near $0°$ C. In this stage, a thin ice shell forms over the drop surface. In the second stage, the drop freezes radially inward at a speed depending on the rate at

which latent heat can be disposed of into the environment, a physical effect that becomes increasingly limited as the ice shell thickens.

For this model formulation, it was assumed that a dendrite formed uniformly during the initial freezing stage, and that the initial freezing time was negligible compared with the freezing time for the second stage. The rate of freezing in the second stage was determined by the heat flux transferred away from the ice shell to the environment. Following the discussion in Pruppacher and Klett (1980) and assuming that inward propagation of the ice shell is radially symmetric, then the energy balance at the water-ice interface may be written as:

$$4\pi\left(1 - \frac{c_w(0 - T_w)}{h_{sf}}\right)\rho_w\, h_{sf}\, r^2 \frac{dr}{dt} = \frac{4\pi\,\lambda_i\, r_o\,(T_0 - T_i(r_o))}{r_o - r}. \qquad (21)$$

The left-hand side of Eq. (21) is the rate of latent heat release due to freezing at the water-ice interface, which is equal to the heat being conducted through the spherical ice shell to the environment, as expressed by the right-hand side of the equation.

The heat being conducted through the ice shell from the water-ice interface (i.e., the inner edge of the ice shell) to the ice-air interface (i.e., the outer edge of the ice shell) is disposed of to the environment by means of convective heat and mass transfer, which is written as:

$$4\pi\,\lambda_i\,(T_0 - T_i(r_o))\frac{r_o\, r}{r_o - r} = 4\pi\, r_o^2\left[\dot{m}''_{subl}\, h_{sg} + h(T_i(r_o) - T_\infty)\right], \qquad (22)$$

where $\dot{m}''_{subl}$ is the rate of mass flux of ice due to sublimation, and h_{sg} is the latent heat of sublimation. The ice shell surface temperature $T_i(r_o)$ was obtained by solving Eq. (22) iteratively. The under-relaxation method of Gerald and Wheatley (1984) was used to improve the rate of convergence. After the surface temperature of the ice shell was determined, the inner

edge of the ice shell (r) was calculated by Eq. (21), while the outer edge of the ice shell (r_0) was calculated using:

$$\frac{dr_o}{dt} = \frac{1}{4\pi r_o^2 \rho_i}\dot{m}''_{subl},$$
(23)

where pi is the density of ice.

Finite Difference Solution of the Heat Diffusion Equation

Because the calculation allowed conditions in the environment air to change at each time step, the unsteady heat diffusion equation (Eq. 1) was solved by the finite difference method. The heat diffusion equation was discretized by the first-order forward time and second-order implicit central space differencing scheme. A set of simultaneous algebraic equations was formed after the discretization. Results from the convective heat and mass transfer analysis provided the boundary conditions for the heat diffusion equations. The resulting system equation for each time step was then solved by the LU decomposition method (Gerald and Wheatley, 1984) to obtain the temperature distribution inside the water drop as a function of time.

Acknowledgments

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