Φ = dimensionless group related to product of Reynolds number and friction factor

Primed quantities are dimensionless.

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Computer Calculation of Binary-Drop Evaporation

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A mathematical model has been developed relating the velocity, temperature, composition, radius, and position of an evaporating drop falling through a heated environment. Under the assumption of rapid mixing within the drop a digital computer program has been written and solved for several initial conditions to give the aforementioned variables as a function of time. Details of the computer program are presented, with emphasis on the analysis of and approach to the problem. The computer results are summarized, and their relation to the general problem of spray vaporization is indicated.

A knowledge of the mechanism of vaporization of liquid drops would add to the over-all understanding of many important chemical and physical processes, such as spray drying, combustion of liquid fuels, and air humidification. To date investigations in these areas have been largely of an experimental nature, involving only single-component drops (*6*, *7*). Verification of an assumed mechanism for a binary-drop vaporization by calculation is difficult because a binary drop is one made up of two distinct components of different volatilities, such that the drop composition changes during evaporation, along with the drop temperature, velocity, direction, and size.

With several simplifying assumptions, summarized in detail by Chinn (*2*), Culverwell (*3*), and Rawson (*9*), two mathematical models have been developed to represent the evaporation of binary drops. The first is called the *rapid mixing* model. It assumes that mass and temperature gradients within the drop are instantaneously removed by convection currents, so that the drop temperature and composition can be represented by average values. This model is approached in larger drops where rapid convection currents are known to exist. The second model assumes no mixing and would be most likely to occur in smaller drops with negligible convection currents. This model requires solution of partial differential equations to determine the temperature and concentration profiles within the drop. The present paper presents the details of a digital computer solution for the rapid mixing model. Computer solution of the no-mixing model is more complicated and is presently under investigation.

PROBLEM ANALYSIS

A system of 37 wt. % tetrachloroethylene, with the remainder orthodichlorobenzene, was chosen for study, since these materials have volatilities similar to those of common jet fuels. Histories of 50- to 400-μ drops were calculated as they evaporated in air at a constant temperature of 600°F. The calculation was begun after the drop was ejected from a nozzle. The initial drop temperature was assumed to be 70°F., the initial velocity 49.5 ft./sec., and the initial trajectory 58.5 deg. to the horizontal.

Calculation of the drop history can be divided into three distinct parts: velocity and trajectory, mass transfer, and heat transfer. The velocity and trajectory equations are derived by applying a force balance to the drop. The resultant force acting on the drop is composed of acceleration due to gravity, the buoyancy effect of the surrounding media, and the frictional resistance of the air.

For the horizontal component of motion

$$m_d\, dv_h/d\theta = -F' \cos\phi \qquad (1)$$

For the vertical component of motion

$$m_d\, dv_v/d\theta = g(\rho_d V_d - \rho_a V_a) - F' \sin\phi \qquad (2)$$

For spheres the frictional force from air resistance is

$$F' = \frac{1}{2}\,(f\, A_x\, \rho_a\, v^2) \qquad (3)$$

Brown (*1*) presents a graphical representation of *f* as a function of the Reynolds number, the curve of which has been approximated analytically by Chinn (*2*) and has been used in the

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present investigation in the following form:

$$N_{Re} < 1.6 \qquad f = 24/N_{Re}$$

$$1.6 \leq N_{Re} < 90 \qquad f = \left(\frac{9{,}000}{N_{Re}^{2}}\right)^{1/3}$$

$$90 \leq N_{Re} < 1{,}000 \qquad f = \left(\frac{100}{N_{Re}}\right)^{1/3}$$

$$N_{Re} \geqq 1{,}000 \qquad f = 0.464$$

The mass transfer equation for one component is

$$dm/d\theta = K(4\pi R^2)(p'_s - p'_{sf}) \quad (4)$$

where K is given by the Ranz and Marshall equation (8):

$$K = (1.0 + 0.3N_{Sc}^{1/3}N_{Re}^{1/2})(Dv\,\rho_f)/R\,(M_m\,p'_a)_{ge} \quad (5)$$

The Ranz and Marshall equation is based on binary diffusion of a pure component in air. The assumption that it holds for ternary diffusion has not been accurately evaluated. However the difference in volatilities of the two components causes binary diffusion to be approached throughout a majority of the evaporation, thus minimizing any error.

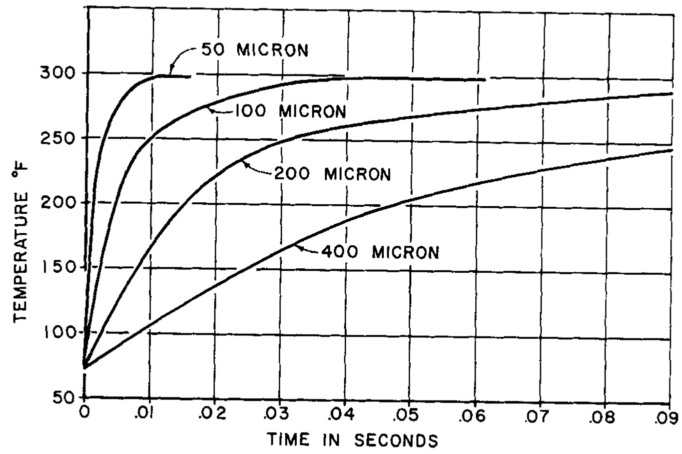

Fig. 2. Temperature histories of binary drops.

The heat transferred to the drop is described by the following equation:

$$dQ/d\theta = h\,4\pi R^2\,(t_a - t_{sav}) \quad (6)$$

Ranz and Marshall (8) give the following expression for the convection heat transfer coefficient:

$$h = k_f\,(1.0 + 0.3N_{Pr}^{1/3}N_{Re}^{1/2}) \quad (7)$$

It should be noted that Equations (5) and (7) were presented by Ranz and Marshall (8) as the result of experiments conducted at atmospheric pressure. The present investigation proposes that their range of applicability be extended to pressures somewhat above atmospheric. Care should be taken to realize that this constitutes an extrapolation with no experimental justification and that trouble may be encountered at pressures greatly different from atmospheric.

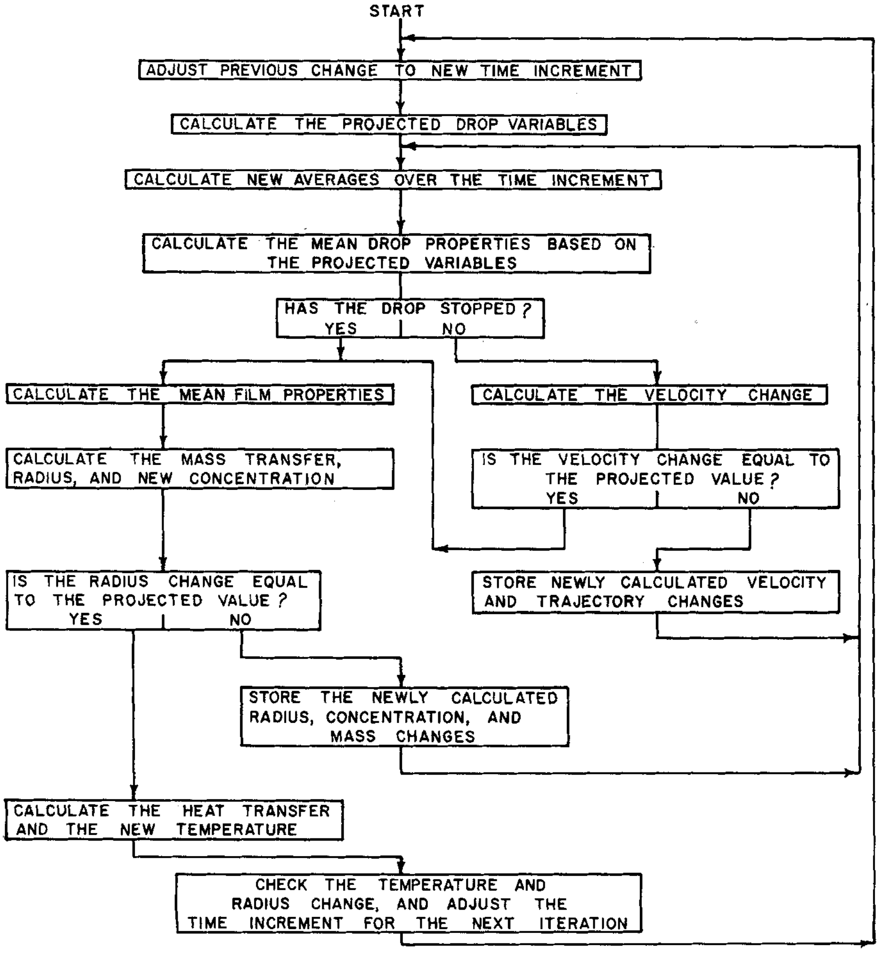

Fig. 1. Summary flow sheet.

COMPUTER PROGRAM

An IBM-650 computer was used for the solution. Since the digital computer must solve differential equations by a step by step finite difference procedure, trial and error must be used. Figure 1 outlines the calculation steps.

All physical and thermodynamic properties, such as the viscosity, specific gravity, friction factor, diffusivity, thermal conductivity, heat capacity, activity coefficient, and heat of vaporization, are expressed as functions of concentration and temperature and are calculated whenever needed. The solution is initiated by choosing a time increment ($\Delta\theta_i$). The time increment is divided by the previous time increment to give a ratio ($\Delta\theta_i/\Delta\theta_{i-1}$). This ratio is used to predict all of the new changes in variables: velocity, trajectory angle, radius, temperature, and concentration. With these newly predicted changes a projected final and average value is calculated for the time increment $\Delta\theta_i$. For example the velocity calculation appears below:

$$\Delta v_i = \Delta v_{i-1}\,(\Delta\theta_i/\Delta\theta_{i-1}) \quad (8)$$

$$v_{av} = v_{i-1} + \frac{1}{2}(\Delta v_i) \quad (9)$$

$$v_i = v_{i-1} + \Delta v_i \quad (10)$$

The differential equations for the velocity change appear below in finite

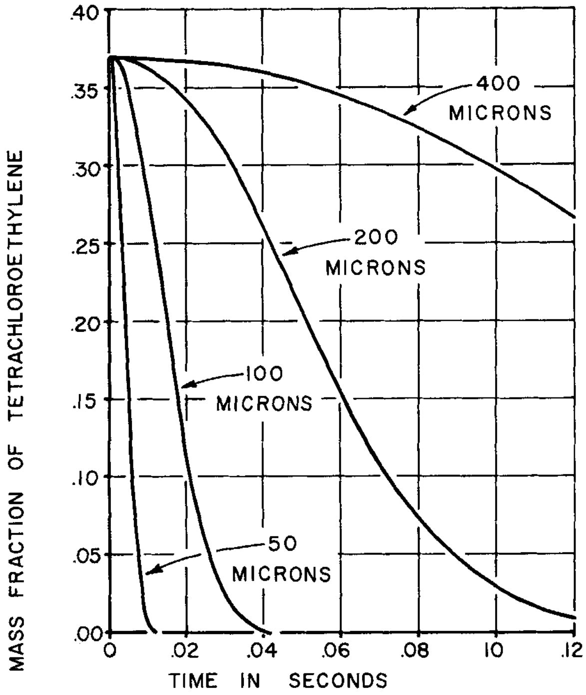

Fig. 3. Concentration histories of binary drops.

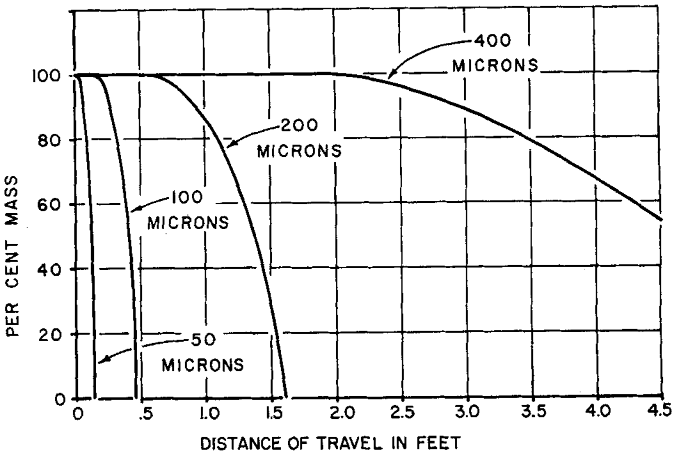

Fig. 4. Mass histories of binary drops.

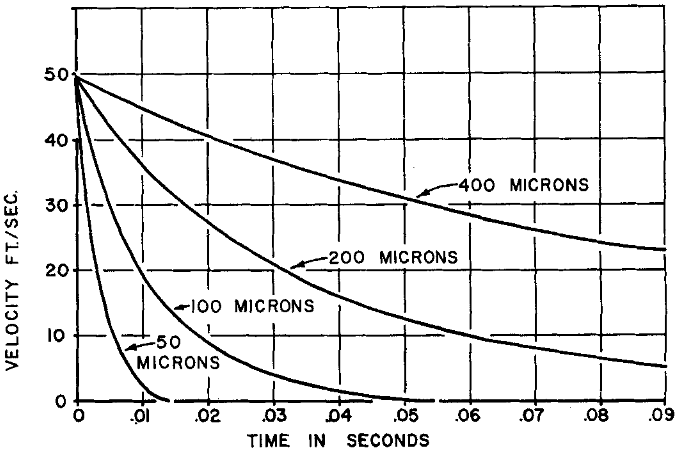

Fig. 5. Velocity histories of binary drops.

difference form and with some rearrangement:

$$\Delta v_{hi} = -CF\, v_i\, \Delta\theta_i \qquad (11)$$

$$\Delta v_{vi} = g\{[(\rho_d - \rho_a)/\rho_d] - CF \sin\phi\}\, \Delta\theta_i \qquad (12)$$

$$\Delta\phi_i = (g \cos \phi_i)\, \Delta\theta_i / v_i \qquad (13)$$

where

$$CF = (3\, f\, \rho_a\, v_i^2)/(8\, g\, \rho_d\, R) \qquad (14)$$

The only assumption in the above equations is that $\rho_d >> \rho_a$. The actual velocity is calculated with the above equations and compared with the projected value. If the projected and calculated values agree within an arbitrary percentage, the program continues. If not the newly calculated values are stored in a place of the projected ones and the calculation repeated until the calculated values equal the previously stored ones. During the calculation all drop properties are calculated as functions of the arithmetic mean temperature and concentration over the time increment. Negligible error is introduced by this if the time increment is kept small.

The mass change over the time increment is determined from the mass transfer equation:

$$\Delta m_i = K_m\, (4\pi\, R^2)\, (p'_s - p'_{sf})\, \Delta\theta_i \qquad (15)$$

The partial pressure at the surface of the vapor film (p'_{sf}) is assumed negligible. This is a good assumption if the drop is moving with a fair velocity. After the mass change is determined, the final radius is calculated as follows:

$$R_i = [(m_{i-1} + \Delta_{mi})/(4\pi\, \rho_d/3)]^{1/3} \qquad (16)$$

As previously with the velocity the difference between the calculated and predicted values of the radius must pass a minimum requirement. If it is not met, the newly calculated values become the predicted ones and the calculations are repeated until the requirement is satisfied. Since the volume is a direct function of the mass, passage of the above velocity and radius tests suffices to accurately fix all variables except temperature.

The temperature is determined by calculating the heat transferred to the drop over the time increment and subtracting the quantity of heat used in vaporizing the mass which has left the drop. The equations are

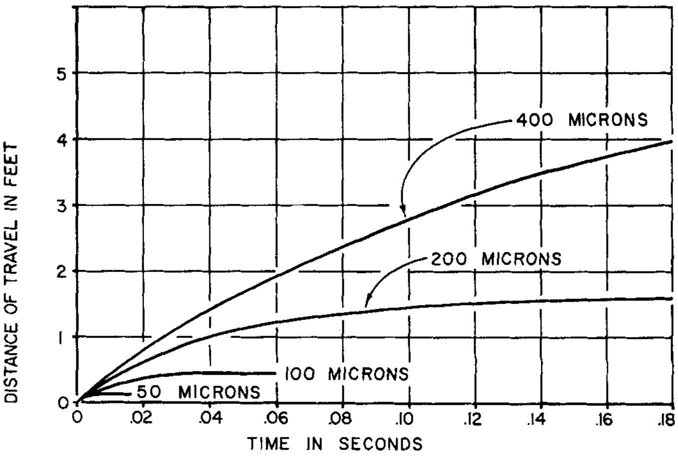

Fig. 6. Movement of binary drops through still air.

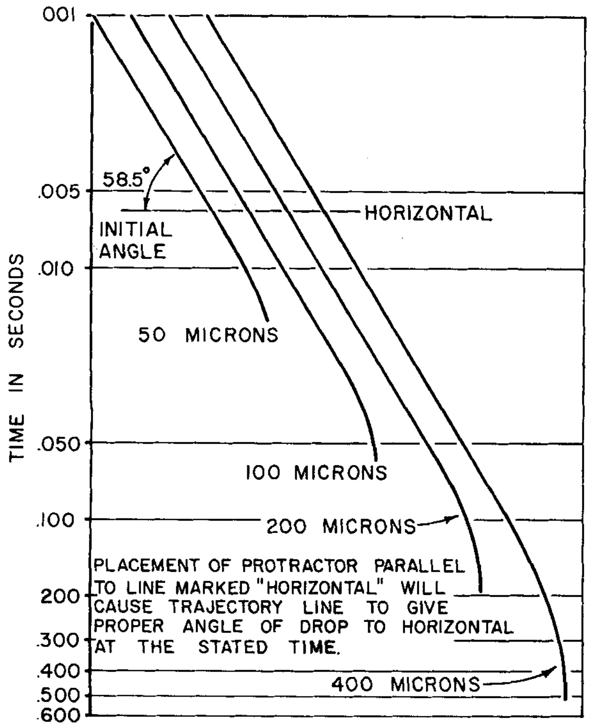

Fig. 7. Drop trajectories.

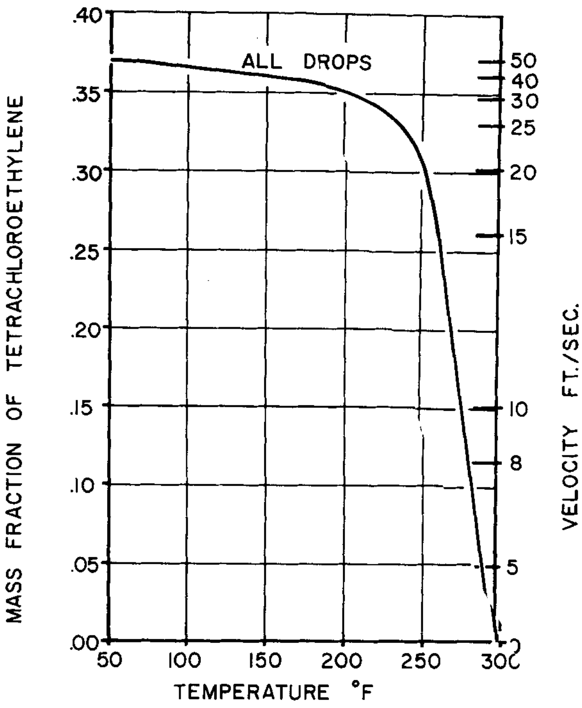

Fig. 8. Combined plots for all sizes of binary drops.

$$\Delta Q_i = h\,4\pi\,R^2(t_a - t_{sav})\,\Delta\theta_i \quad (17)$$

$$t_{dav} = Q_{\text{net}}/m_i\,C_{pd} \quad (18)$$

Radiation effects were found negligible and were not considered (*2*). The mass of each component evaporated is subtracted from the amount previously present, and the result is divided by the new drop mass to determine the new average concentration. No concentration and temperature profile calculations are necessary, since instantaneous mixing has been assumed and the entire drop is represented by average values.

The final check is a temperature change and time increment test so that the trial-and-error solution will remain accurate. This is accomplished by adjustment of the time increment for the next iteration so that changes will occur slowly. This allows representation of the drop properties by averages over the time increment without sacrificing accuracy.

Possible changes in air temperature and composition during evaporation have not been taken into account for two reasons. First the calculations presented here apply to a single binary drop falling through a heated environment. Such a drop is continually encountering fresh air of constant temperature and composition. Second to extend the results of such calculations to a spray made up of many drops it is only necessary to specify that the spray be subjected to a continuous supply of pure air at constant temperature. In most cases this can be done with little difficulty by means of some air feeding device. In either case the simplicity of the resulting system of equations makes the assumption of constant temperature and composition desirable.

RESULTS

The time for solution on the computer varied from ½ hr. for the 50-μ drop to over 2 hr. for the 400-μ drop. Figures 2 through 8 summarize the results of 50-, 100-, 200-, and 400-μ drops. The temperature histories of the drops present a consistent family of curves which all reach an equilibrium temperature of 298°F. (Figure 2). The 200- and 400-μ drops are not completely displayed owing to scaling, but they also reached 298°F. Reference to the concentration histories (Figure 3) shows that the equilibrium values are obtained just after the tetrachloroethylene concentration becomes zero. This is expected since the drop is now pure orthodichlorobenzene and will reach an equilibrium temperature somewhat below its boiling point of 357°F.

Ingebo (*6*) studied eight pure drops evaporating at variety of temperatures. He presented an empirical equation for the equilibrium (wet-bulb) temperature as a function of boiling point and air temperature. For orthodichlorobenzene in air at 600°F. this equation gives 260°F. for the equilibrium temperature, which is somewhat low. However the only compound Ingebo investigated with a boiling point comparable to that of orthodichlorobenzene was nitrobenzene (B.P. 412°F.) It exhibited an equilibrium (or wet-bulb) temperature approximately 72°F. below its boiling point, which is comparable to the 57°F. decrease predicted for orthodichlorobenzene by the present study.

The remaining figures show very consistent families of curves displaying all of the drop variables. All drops approach the equilibrium temperature as the velocity approaches zero (Figures 2 and 5). A drop could not reach an equilibrium state with a finite velocity, since any further evaporation would cause the velocity to change.

Figures 4 and 6 show that a large portion of the mass evaporated with little change in distance. As much as 50% of the smaller drops evaporated after the velocity approached zero. This occurs since the drop is relatively cool during the higher velocities. Figure 7 shows that the 50-μ drop disappeared so quickly that it essentially lost its momentum instantaneously and did not have sufficient time to swing into a vertical trajectory.

It is interesting to note from Figures 2, 3, and 5 that drops at identical temperatures have the same velocity and concentration. Figure 8 presents one curve which correlates all the drop variables. All drops went through identical histories upon evaporating, the only difference being time. Further investigation shows that doubling the diameter of the drop maintains the same history but displaces the variables in time by a factor of 3.2. If one assumes the time increase is directly proportional to the mass and inversely proportional to the surface area, doubling the diameter would double the time. Without further investigation the only conclusion is that mass apparently affects the time more than the surface area.

An attempt has been made to compare the results of the present investigation with those of El Wakil, Uyehara, and Meyers (4). Unfortunately, owing to the use of different basic assumptions, only a qualitative comparison can be made, but the results of the two studies do appear to be consistent. It seems to the present authors that the effect of mass transfer on heat transfer can be safely neglected because of the prior assumption that the air temperature and composition remain unchanged throughout the vaporization process (made by both sets of investigators). In the process of deriving their correction factor for mass transfer El Wakil et al. consider the term θ_s, the heat carried out with the diffusing vapor in the form of superheat. This term has a significant value because they assume that the vapor is heated up to the temperature of the surrounding air by the time it leaves the film. In the light of the previous assumption that the air temperature remains unchanged, such a large superheat is unlikely. There is just not time for the necessary heat transfer to the vapor to take place. In the present calculation the opposite extreme was assumed, that the vapor moved through the film and was swept away so rapidly that no superheating took place. Both assumptions are inexact, but it is believed that the present assumption of no superheating is closer to the truth; that is it seems likely that the vapor leaving the film surrounding the droplet will be closer to the droplet surface temperature than to the temperature of the surrounding air.

CONCLUSIONS

Little experimental work has been done to substantiate the results of this calculation. Studies previous to this work were conducted at Northwestern University (3) by spraying orthodichlorobenzene and tetrachloroethylene into a heated chamber and collecting the drops at various levels in trays of liquid nitrogen. The only comparable data available indicated that the distances of travel were of the same magnitude as those predicted by the calculation. Experiments of this nature are difficult to conduct owing to the rapid convection currents caused by the heated chamber and the liquid nitrogen. Future work should be directed toward experimental verification of the rapid mixing model. If it proves adequate, the approach would be invaluable to fuel vaporization, spray drying, humidification, and similar studies.

The following relationship was found for the drop histories:

$$\theta_1/\theta_2 = (R_1/R_2)^{1.68} \qquad (19)$$

Since all the drops were found to go through identical histories displaced in time, Equation (19) allows calculation of any size drop history if the history of one size drop is known. Any pure component or binary-drop system can be evaluated by this program with comparative ease. Thus if the rapid mixing model proves adequate, a drop-size distribution would be all that is required to completely evaluate the behavior of atomization equipment.

It should be pointed out that an expression much like Equation (19) has been previously determined experimentally by Ingebo (5). His exponent was 1.84, however which is not far from the value of 1.68 proposed as the result of the present investigation. Further studies may bring the two exponents even closer together.

SUMMARY

Histories of 50-, 100-, 200-, and 400-μ drops composed of tetrachloroethylene and orthodichlorobenzene were calculated on the digital computer as they evaporated in air. Velocity, radius, temperature, composition, and position were determined as a function of time. A rapid mixing model was assumed so that temperature and concentration gradients within the drop could be represented by average values. It was found that all drop sizes go through identical histories, but displaced in time. The ratio of times was proportional to the ratio of the radii to the 1.68 power. Experimental work is needed to evaluate the accuracy of the model. If the model is adequate, this approach can be very valuable in the design of industrial equipment.

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NOTATION

A = area
C_p = heat capacity, constant pressure
CF = common factor, $(3\rho_a f v^2/8 g \rho_L R)$
d = differential
D_v = diffusivity of the vapor
f = friction factor
F' = resisting force of air friction
g = acceleration of gravity
h = convection heat transfer coefficient
k = thermal conductivity
K = mass transfer coefficient
m = mass
M = molecular weight
N_{Pr} = Prandtl number, $(C_{Pa}\mu_a/kf)$
N_{Re} = Reynolds number, $(\rho_a 2Rv/\mu_a)$
N_{Sc} = Schmidt number, $(\mu_a/\rho_a D_f)$
p' = partial pressure
Q = heat transferred
R = drop radius
t = temperature
v = velocity
V = volume
θ = time
μ = viscosity
ρ = density
ϕ = angle of trajectory

Subscripts

a = air
av = average over time increment $\Delta\theta$
d = drop
f = film
ge = geometric mean
h = horizontal
i = component i
i = present time increment
$i-1$ = previous time increment
m = arithmetic mean average based on mass or mole fraction.
s = surface of drop
sf = surface of film surrounding drop
v = vertical
x = cross sectional

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