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## SUFFIELD TECHNICAL PAPER

NO. 376

LIQUID DROP ABSORPTION AND EVAPORATION FROM A SUBSTRATE

THE VARYING SURFACE AREA MODEL (U)

bу

R.S. Weaver

PROJECT NO. 20-20-32

July 1972



DEFENCE RESEARCH ESTABLISHMENT SUFFIELD: RALSTON: ALBERTA

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## LIQUID DROP ABSORPTION AND EVAPORATION FROM A SUBSTRATE THE VARYING SURFACE AREA MODEL (U)

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R.S. Weaver

### **ABSTRACT**

This paper continues the development of physical and mathematical models applicable to liquid drop absorption and evaporation from a substrate. Three examples are considered: a constant radius of curvature model; a constant base area model; and a constant angle of contact model. All allow the free surface area of the drop to vary with time. Methods of solution are given for both monodisperse and polydisperse drop distributions, and the results are compared with experimental data. Both the constant radius of curvature and constant angle of contact versions provide reasonable fits to experiment.

## RÉSUMÉ

Ce document continue le développement des modéles physiques et mathématiques applicables à l'absorption de chute liquide et à l'evaporation d'un substratum. Trois exemples sont considérés: un modèle à rayon de courbure constant; un modèle à aire de base constante; et un modèle à angle de contact constant. Tous les trois permettent l'aire superficielle libre de la chute de varier avec le temps. Des méthodes de solution sont proposées pour toutes les deux distributions à chute - monodisperse et polydisperse, et les résultats sont comparés aux données expérimentales. Les modèles à rayon de courbure constant et à angle de contact constant fournissent des versions qui s'accordent raisonnablement avec l'expérience.

## DEFENCE RESEARCH ESTABLISHMENT SUFFIELD RALSTON ALBERTA

### SUFFIELD TECHNICAL PAPER NO. 376

# LIQUID DROP ABSORPTION AND EVAPORATION FROM A SUBSTRATE THE VARYING SURFACE AREA MODEL

bу

R.S. Weaver

#### INTRODUCTION

The history of a dispersion of drops of a liquid which has fallen on vegetation or soil was examined in previous reports (1,2). Drop behaviour, applied particularly to pick-up, was discussed in one of these reports (2) in light of a simulation called the constant area disc model. This model was found useful in laboratory conditions and in certain special field situations. Also, the equations developed from the model was analytically soluble and were helpful in examining gross characteristics of drop behaviour. However, the theoretical equations for drop evaporation and pick-up gave a poor fit to the results from field experiments on prairie grassland; consequently, alternative models were developed and will be described below. Again the models will use as a starting point the idealized case of discrete droplets on a smooth plane surface.

The common characteristic of the following models is the variation of the surface area of a drop with time. This variation leads to differential equations for evaporation, absorption, etc., which are in many cases only digitally soluble. Consequently, after the system equations for each of the special cases considered have been derived, any numerical methods of solution required in the digital computer programs will also be outlined. The equations obtained to describe a single drop will apply, with a constant factor, to a monodisperse drop distribution; polydisperse distributions have to be considered somewhat differently. An extension of some of the numerical methods used for monodisperse distributions will be described for the solution of the system equations for polydisperse drops.

The equations for monodisperse drops have also been solved directly by analog computer; this method will not be described in detail, since it is relatively straightforward. The analog computer is most useful as a check on the digital approach, since it is too slow for generation of large tables of results, or for investigating many parameter changes.

Specific flow charts and programs for digital and analog solutions of the system equations for one of the models are given as an example in Appendix II. These computer programs are readily convertible to obtain solutions to the equations of other models by simply substituting the appropriate differential or analytic expressions in the FORTRAN program.

### GENERAL EXPERIMENTAL FEATURES

Experimentally observed facets of drops and their distributions are discussed more fully in previous reports (1,2), and will only be summarized here. As before, the models assume liquid drops deposited without overlap on a uniform smooth plane.

One parameter appearing in the following sections is the spread factor  $\lambda$ , defined as the ratio of  $A_0$ , the base diameter of the drop on the substrate, to D, the original diameter of the free liquid drop. The best fit of theory to experiment results when  $\lambda$  is in the range of 3 to 5 for drops on prairie vegetation.

Several of the constants which appear in the following derivations may in fact be functions of meteorological conditions, drop size, etc. Examples are the liquid drop evaporative coefficient  $\mathbf{C}_1$  and absorptive coefficient  $\mathbf{C}_2$ . In this report, the simplifying assumption is made that such coefficients are constants during the course of an experiment.

Models of drop behaviour are considered for both monodisperse (drops of one diameter) and polydisperse (drops of a range of diameters) distributions. In particular, the polydisperse distribution function considered will be a Pearson Incomplete  $\Gamma$ -function distribution <sup>(3)</sup>; this has been experimentally found <sup>(4)</sup> to predict satisfactorily the distribution of drop sizes from devices such as an agricultural boom sprayer. Experimental results of field trials to measure absorption, evaporation and liquid pick-up from the substrate, both for monodisperse and polydisperse drop distributions, are available and will be compared with the model predictions.

## THEORY OF A VARYING SURFACE AREA MODEL

Consider a spherical drop of radius  $r_0$  falling on a surface, and spreading into the shape of a section of a sphere (Figure 1). If R is the radius of curvature of the spherical surface, h the height at the centre of the drop, and a the radius of the base, then the drop volume is

Now the initial volume  $V_0 = \frac{4}{3} \pi r_0^3$ , where  $r_0$  is the original free drop radius.

Hence 
$$\frac{4}{3} \pi r_0^3 = 1/6 \pi h_0 (h_0^2 + 3a_0^2) - - - - - - - - - - - - - - - - - (5)$$

(where  $h_0$  and  $a_0$  are initial values of h and a)

or 
$$h_0^3 + 3a_0^2 h_0 - 8r_0^3 = 0$$
 ---- (5a)

Let  $a_0 = \lambda r_0$ , where  $\lambda = \text{spread factor.}$ 

Solving equation (6) for h leads to

$$h_o = \{ [4 + (16 + \lambda^6)^{\frac{1}{2}}]^{1/3} + [4 - (16 + \lambda^6)^{\frac{1}{2}}]^{1/3} \} r_o - - - - (7)$$

= 
$$Kr_0$$
, where  $K = f(\lambda) - - - - - - - - - - - - - (7a)$ 

Substituting in equation (1) gives

Now the liquid in the spread drop will disappear by absorption by the substrate and by evaporation. Assume that evaporation is proportional to the drop free surface area  $\mathbf{A}_{\mathbf{s}}$ , and absorption is proportional to the drop base area.

where  $C_1$  and  $C_2$  are evaporative and absorptive coefficients.

Equations (1) or (2) and (9) lead to only two independent equations involving h, R and a. In order to solve these equations, one of the three variables, or a ratio of two of them, must be considered as a constant. As the drop disappears, its height h will almost certainly decrease; hence either R or a could be held constant. In addition, the angle of contact  $\alpha$  (see Figure 1) may remain constant as the drop disappears. These possibilities will be analyzed in the following sections.

(i) Constant radius of curvature R -

Differentiating (1) gives

$$\frac{dV}{dt} = \pi h (2R-h) \frac{dh}{dt} - - - - - - - - - - - - - - - - - (10)$$

Substituting (10) and (3) in (9),

$$\pi h(2R-h) \frac{dh}{dt} = -C_1(2\pi Rh) - C_2\pi h(2R-h)$$

$$dh \frac{2C_1R}{2}$$

Now assume that absorption can be considered as similar to diffusion into a semi-infinite medium following a step input boundary condition (2). Then the absorptive rate will be proportional to  $t^{-\frac{1}{2}}$ ; that is,  $C_2$  must be replaced by

Then 
$$\frac{dh}{dt} = -2 \frac{C_1 R}{2R-h} - \frac{C_2}{\sqrt{t}}$$
 ---- (12)

where  $h_0 (\equiv h(o))$  is given by equation (7), and  $R = R_0$  by equation (8).

For solution, put  $x = \sqrt{t}$  and y = 2R-h; then dt = 2xdx and dy = -dh.

Equation (12) becomes

To solve, put  $\frac{x}{y} = V$ ; then dx = ydV + Vdy.

Put 
$$4C_1R = A; 2C_2 = B$$

Then dy = (AV + B) (ydV + Vdy)

This equation may be solved for y and V. Then substitution for V, A and B leads finally to

$$\left[\frac{y^2 - 2C_2 xy - 4RC_1 x^2}{y_0^2}\right]^{\frac{1}{C_2}} = \left[\frac{C_2}{2RC_1} \left\{ \left(C_2^2 + 4RC_1\right)^{\frac{1}{2}} - C_2 \right\} - 1 \right].$$

$$\left[\frac{4RC_{1}x+y[C_{2}+(C_{2}^{2}+4RC_{1})^{\frac{1}{2}}]}{4RC_{1}x+y[C_{2}-(C_{2}^{2}+4RC_{1})^{\frac{1}{2}}]}\right] - - - - - - - - - - - - - - - (15)$$

Here y is not obtained as an explicit function of x (ie,  $t^2$ ); for any given time, determination of y is anything but straighforward. Some method of numerically solving for y, such as the Newton-Raphson method, must be employed. This would involve the derivative of equation (15) with respect to y. This was done, and the solution obtained by digital computer. However, the entire procedure is algebraically untidy; consequently it was also decided to attempt direct integration of the differential equation (13) by numerical methods. Since the starting value of y and the equation for its first derivative are known, a fourth order Runge-Kutta integration procedure was used. These numerical techniques will be more fully described later.

The quantities of interest in considering the behaviour of a drop on a substrate are the amounts of liquid evaporated, absorbed by the substrate and remaining in the substrate. Let these quantities by  $Q_{\rm E}$ ,  $Q_{\rm A}$  and  $Q_{\rm AR}$  respectively.

Then the rate of evaporation will be

$$\frac{dQ_E}{dt} = C_1 (2\pi Rh) ----- (16)$$

Similarly, 
$$\frac{dQ_A}{dt} = \frac{C_2}{\sqrt{t}} \pi h$$
 (2R-h) ----- (17)

Now assume that the liquid absorbed by the substrate becomes unavailable or decays (due to chemical decomposition, etc.) at some rate  $\epsilon$ .

Then 
$$\frac{dQ_{AR}}{dt} = \frac{C_2}{\sqrt{t}}$$
  $\pi h (2R-h) - \epsilon Q_{AR}$  ---- (18)

Writing 2R-h = y and  $\sqrt{t} = x$ ,

$$\frac{dQ_{A}}{dx} = 2\pi C_{2}y(2R-y) -----(20)$$

$$\frac{dQ_{AR}}{dx} = 2\pi C_2 y (2R - y) - 2\varepsilon x Q_{AR} - - - - - - - - - - (21)$$

For each value of x, y is known from solving (14) or (15). Consequent1 (19) and (20) may be solved by Runge-Kutta formulae. Alternatively, since values of  $Q_E$  and  $Q_A$  at each previous time are known, these equations are soluble by Newton-Cotes numerical integration formulae of the closed type. Both methods wer tried, and are discussed later. No significant difference was noted in either computer time or accuracy.

Since the derivative of  $Q_{\mbox{AR}}$  involves  $Q_{\mbox{AR}}$  itself (equation (21)), none of the previous numerical methods are directly applicable. Here a predictor-correct method was used, as discussed below.

When all of these quantities have been determined, the pick-up of liquifrom the substrate by a pad or roller can be determined. The amount of pick-up will be a fraction of the remaining free liquid plus another fraction of the absorbed liquid, some of which will be expressed by the weight of the roller.

(ii) Constant base area - From a =  $\lambda r$ , a may be calculated (for notational convenience, put a $\equiv$ a)

Now from equation (3),

$$R = \frac{a^2 + h^2}{2h}$$

Substituting for R in equation (9) gives

$$\frac{dV}{dt} = -\pi C_1 h^2 - (C_1 + \frac{C_2}{\sqrt{t}}) (\pi a^2) - - - - - (22)$$

And from equation (2),

$$\frac{dV}{dt} = \frac{\pi}{2} (h^2 + a^2) \frac{dh}{dt}$$

Therefore, 
$$\frac{\pi}{2} (h^2 + a^2) \frac{dh}{dt} = -\pi C_1 h^2 - (C_1 + \frac{C_2}{\sqrt{t}}) \pi a^2$$

$$\frac{dh}{dt} = \frac{2C_1h^2}{h^2 + a^2} - 2(C_1 + \frac{C_2}{t}) \frac{a^2}{h^2 + a^2} = -2C_1 - \frac{2C_2}{\sqrt{t}} \frac{a^2}{h^2 + a^2} - -(23)$$

As before, put  $\sqrt{t} = x$ ; then dt = 2xdx

Therefore, 
$$\frac{dh}{dx} = -4C_1x - 4C_2 \left(\frac{a^2}{h^2 + a^2}\right) - - - - - - - - (24)$$

No analytic solution was found for this equation; however, it can be solved readily by the Runge-Kutta method.

As before,

$$\frac{dQ_{AR}}{dt} = \pi C_2 \frac{a^2}{\sqrt{t}} - \epsilon Q_{AR} - - - - - - - - - - - - - - - - - - (27)$$

Letting  $\sqrt{t} = x$  leads to

$$\frac{dQ_E}{dx} = 2\pi C_1(a^2 + h^2)x - \frac{1}{2} - - - - - - - - - - - - - - (28)$$

Now equation (28) is soluble again by Newton-Cotes or Runge-Kutta formulae.

Solving equation (29) gives

$$Q_{A} = 2\pi C_{2} a^{2} x$$

$$= 2\pi C_{2} a^{2} \sqrt{t}$$

This is an analytic expression which gives  $\mathbf{Q}_{\mathbf{A}}$  explicitly. Similarly, equation (30) gives

$$Q_{AR} = 2\pi C_2 a^2 e^{-\epsilon x^2} \int_0^x e^{\epsilon x^2} dx ---- (32)$$

Unfortunately, this solution is given in terms of Dawson's Integral  $^{(6)}$ , and must be numerically evaluated. Hence the analytic solution is of little advantage, and equation (30) was again solved by a predictor-corrector technique.

## (iii) Constant angle of contact $\alpha$

From Figure 1, the angle of contact  $\alpha$  between the drop and the substrate is also equal to half the angle subtended at its centre of curvature by the spherical segment. If the angle  $\alpha$  remains constant, then so does cos  $\alpha$ ;

ie, 
$$\cos \alpha = \frac{R-h}{R} = 1 - \frac{h}{R}$$
 is constant.   
Or,  $1 - \frac{h}{R} = 1 - \frac{h_o}{R_o}$    
 $\frac{h}{R} = \frac{h_o}{R_o}$    
and  $R = \frac{R_o}{h_o}$  h

Now from equations (7a) and 8,  $\frac{R_o}{h_o} = \frac{4 + K^3}{3K^3}$ 

Hence R = 
$$\left[\frac{4 + K^3}{3K^3}\right]$$
 h  
= Bh, where B =  $\frac{4 + K^3}{3K^3}$  ---- (33)

Let  $Q_E$  = quantity of liquid evaporated,  $Q_A$  = quantity absorbed by substrate,  $Q_{AR}$  = quantity remaining in substrate.

The equations previously derived for these quantities are:

Also as before, from Equation (9),

Substituting in (1), 
$$V = \frac{1}{3}\pi h^3(3 B-1) - - - - - - - - - - - (34)$$

$$. . . \frac{dV}{dt} = \pi h^2 (3B-1) \frac{dh}{dt} - - - - - - - - - - - - - - - - - (35)$$

Equation (9a) becomes

$$\frac{dV}{dt} = -C_1(2\pi Bh^2) - \frac{C_2\pi}{\sqrt{t}}h^2 (2B - 1) - - - - - - - - - (36)$$

Equating (35) and (36) gives

$$\pi h^2 (3B - 1) \frac{dh}{dt} = -2\pi BC_1 h^2 - \frac{\pi (2B - 1)C_2}{\sqrt{t}} h^2$$

or 
$$\frac{dh}{dt} = \frac{-2BC_1}{3B-1} - \frac{(2B-1)C_2}{(3B-1)\sqrt{t}}$$
 ---- (37)

 $Put\sqrt{t} = x; then dt = 2xdx$ 

Then 
$$\frac{dh}{dx} = -\frac{4BC_1}{3B-1} \times -\frac{2(2B-1)C_2}{3B-1}$$
 ----(38)

Put H = 
$$\frac{h}{h_o}$$
  
m =  $\frac{2BC_1}{h_o (3B-1)}$ 

$$n = \frac{2(2B-1)}{3B-1} \frac{C_2}{h_0}$$

Then 
$$\frac{dH}{dx} = -2mx - n$$
 - - - - - - - - - - - - (38a)

. H = Const. 
$$-mx^2 - nx$$
  $-----$  (39)

At t = 0 (or x = 0), H = 
$$\frac{h_0}{h_0}$$
 = 1

. . 
$$H = 1 - mx^2 - nx$$
 ---- (39a)

or 
$$h = (1 - mt - nt^{\frac{1}{2}})h_0$$
 ---- (39b)

Now from (16), 
$$\frac{dQ_E}{dt} = 2\pi BC_1 h^2$$

= 
$$2\pi BC_1h_0^2 (1 - mt - nt^{\frac{1}{2}})^2 - - - - - - - (40)$$

or 
$$Q_E = 2\pi BC_1h_0^2 \left[\frac{1}{3}m^2t^3 + \frac{4}{5}mnt^{5/2} + \frac{1}{2}(n^2 - 2m)t^2 - \frac{4}{3}nt^{3/2} + t\right] --(40a)$$

Here the constant of integration = 0.

Normalizing with respect to  $V_{o}$  (Eqn. 34) gives

$$\frac{Q_E}{V_o} = \frac{2\pi B C_1 h_o^2}{\frac{1}{3} \pi h_o^3 (3B-1)} f_1(t) = \frac{6BC_1}{h_o(3B-1)} f_1(t) = 3mf_1(t) - - - - (41)$$

where  $f_1(t)$  is the expression in brackets in (40a).

From (17) and (3), 
$$\frac{dQ_A}{dt} = \pi C_2$$
 (2B-1)  $h^2 t^{-\frac{1}{2}}$ 

$$= \pi C_2 (2B-1)h_0^2 [m^2 t^{3/2} + 2mnt +$$

$$(n^2 - 2m)t^{\frac{1}{2}} - 2n + t^{-\frac{1}{2}}] - - - - - - (42)$$

Then 
$$Q_A = \pi C_2 (2B-1) h_o^2 \left[\frac{2}{5}m^2t^{5/2} + mnt^2 + \frac{2}{3}(n^2 - 2m)t^{3/2}\right]$$

$$-2nt + 2t^{\frac{1}{2}}$$
 ---- (42a)

(Again constant of integration = 0).

Normalizing, 
$$\frac{Q_A}{V_o} = \frac{C_2(2B-1) h_o^2}{\frac{1}{3} h_o^3 (3B-1)} f_2(t) = \frac{3C_2(2B-1)}{h_o(3B-1)} f_2(t)$$
  
= 1.5 nf<sub>2</sub>(t) - - - - - - - - - - - - - (43)

where  $f_2(t)$  is the bracketed expression in (42a).

Eqn. (18) gives

$$\frac{dQ_{AR}}{dt} = \frac{dQ_A}{dt} - \epsilon Q_{AR} = f_3(t) - \epsilon Q_{AR} - - - - - - - - - - (43)$$

where  $f_3(t)$  is the right hand side of (42).

In standard form,  $\frac{dQ_{AR}}{dt} + \epsilon Q_{AR} = f_3(t)$ 

The solution is 
$$Q_{AR} = e^{-\varepsilon t} \int_{0}^{t} f_3(t^1)e^{\varepsilon t^1} dt^1 + Const. \cdot e^{-\varepsilon t} --(44)$$

Here 
$$f_3(t) = \pi C_2 (2B-1) h_0^2 [m^2 t^{3/2} + 2mnt + (n^2-2m) t^{\frac{1}{2}} -2n + t^{-\frac{1}{2}}]$$

Put 
$$a_0 = \pi C_2$$
 (2B-1)  $h_0^2$ ;  $a_1 = m^2$ ;  $a_2 = 2mn$ ;  $a_3 = n^2 - 2m$ ;  $a_4 = -2n$ 

Then 
$$f_3(t) = a_0 (a_1 t^{3/2} + a_2 t + a_3 t^{\frac{1}{2}} + a_4 + t^{-\frac{1}{2}})$$

$$Q_{AR} = a_0 e^{-\varepsilon t} \int_0^t \left[ a_1(t^1)^{3/2} + a_2(t^1) + a_3(t^1)^{\frac{1}{2}} + a_4 + (t^1)^{-\frac{1}{2}} \right]^{\frac{1}{2}}$$

$$e^{\varepsilon t^1} dt^1 + Const. \cdot e^{-\varepsilon t}$$

Integrating by parts and collecting terms,

In the integral expression, let  $\sqrt{\varepsilon t^1} = u$ .

Then 
$$t^1 = \frac{u^2}{\varepsilon}$$
 and  $dt^1 = \frac{2udu}{\varepsilon}$ 

Put  $\sqrt{\epsilon t} = z$ ; then last term becomes

$$\left(1 - \frac{a_3}{2\varepsilon} + \frac{3a_1}{4\varepsilon^2}\right) \sqrt{\frac{2}{\varepsilon}} \left[ e^{-z^2} \int_0^z e^{u^2} du \right]$$

The last bracketed expression is Dawson's integral and is calculable or tabulated in handbooks.

Hence

$$Q_{AR} = a_{o} \left\{ \frac{1}{\varepsilon} \left[ a_{1} t^{3/2} + a_{2} t + \left( a_{3} - \frac{3a_{1}}{2\varepsilon} \right) t^{\frac{1}{2}} + \left( a_{4} - \frac{a_{2}}{\varepsilon} \right) \right] + \frac{2}{\sqrt{\varepsilon}} \left( 1 + \frac{a_{3}}{2\varepsilon} + \frac{3a_{1}}{4\varepsilon^{2}} \right) \cdot DI \right\} + Const. \cdot e^{-\varepsilon t} - - - - (46)$$

(where DI = Dawson's integral

$$= e^{-z^2} \int_0^z e^{u^2} du, z = \sqrt{\varepsilon t}$$

Normalizing, 
$$\frac{Q_{AR}}{V_o} = \frac{a_o}{V_o} f_{\downarrow}(t) = \frac{\pi C_2 (2B-1) h_o^2}{\frac{\pi}{3} h_o^3 (3B-1)} f_{\downarrow}(t) = 1.5 n f_{\downarrow}(t)$$

where  $f_{h}(t)$  is given in the curly brackets of (46).

### NUMERICAL SOLUTION TECHNIQUES

#### (i) Solution for h -

Equations (13) and (24), which are differential equations for h as a (5) function of time, were solved by a standard fourth order Runge-Kutta procedure (5). If the first derivative at  $\mathbf{x}_n$ ,  $\mathbf{y}_n$  is given by  $\mathbf{f}(\mathbf{x}_n, \mathbf{y}_n)$  where  $\mathbf{x}_n$  is the independen variable, then  $\mathbf{y}_{n+1}$  at  $(\mathbf{x}_n + \Delta \mathbf{x})$ , where  $\Delta \mathbf{x}$  = step size, is given by

$$y_{n+1}(x+\Delta x) = y_n(x) + \frac{1}{6} (K_1 + 2K_2 + 2K_3 + K_4) + 0(\Delta x^5);$$
Here
$$K_1 = \Delta x \ f(x_n, y_n)$$

$$K_2 = \Delta x \ f(x_n + \frac{1}{2}\Delta x, \ y_n + \frac{1}{2} K_1)$$

$$K_3 = \Delta x \ f(x_n + \frac{1}{2} \Delta x, \ y_n + \frac{1}{2} K_2)$$

$$K_4 = \Delta x \ f(x_n + \Delta x, \ y_n + K_3)$$

The dependent variable y was also computed at  $\mathbf{x}_n + \frac{1}{4} \Delta \mathbf{x}$ ,  $\mathbf{x}_n + \frac{1}{2} \Delta \mathbf{x}$  and  $\mathbf{x}_n + \frac{3}{4} \Delta \mathbf{x}$ , for use in calculating  $\mathbf{Q}_E$  and  $\mathbf{Q}_A$ , as outlined below.

## (ii) Solutions for $Q_A$ and $Q_E$ -

Equations (19) and (28) for  $Q_E$  and (20) for  $Q_A$  were computed by the Runge-Kutta routine, and by using a Newton-Cotes integration formula of the closed type<sup>(5)</sup>. This can be written in the following form, where again  $\Delta x$  is the step size:

$$y_{n+1} (x + \Delta x) = y_n(x) + \frac{\Delta x}{90} [7y^1(x + \Delta x) + 32y^1(x + 3/4 \Delta x) + 12y^1(x + \frac{1}{2}\Delta x) + 32y^1(x + \frac{1}{2}\Delta x) + 7y^1(x)] + 0(\Delta x^7) - (49)$$

$$y^1(x) = \frac{d}{dx} y(x)$$

Since each  $y^1$  is a function of time and the equivalent h, the values of h at intermediate steps between x and  $x+\Delta x$  are obtained from the previous step to compute the required derivative values.

## (iii) Solutions for $Q_{AR}$ -

where

Equations (21) and (30) were solved by a predictor-corrector method. Let QAR be the amount absorbed remaining, DQAR be its derivative with respect to the independent variable; let QA and DQA be the amount absorbed and its derivative respectively.

Now from equation (21),

$$DQAR(x) = 2\pi C_2 y(2R-y) - 2\epsilon xQAR(x)$$

But from (20),

$$2\pi C_2 y(2R-y) = DQA(x)$$

Hence 
$$DQAR(x) = DQA(x) - 2\varepsilon xQAR(x) - - - - - - - - - - - (50)$$

and 
$$DQAR(x + \Delta x) = DQA(x + \Delta x) - 2\varepsilon(x + \Delta x) QAR(x + \Delta x) - - - - (51)$$

Now the trapezoidal rule (5) is

$$QAR(x + \Delta x) = QAR(x) + \frac{\Delta x}{2} \left[ DQAR(x + \Delta x) + DQAR(x) \right] - - - - (52)$$

However, DQAR(x +  $\Delta$ x) from equation (36) also contains QAR(x +  $\Delta$ x). Hence the procedure is to assume an initial value for QAR(x +  $\Delta$ x), substitute this value in equation (36) to obtain an estimate of DQAR(x +  $\Delta$ x), and substitute this again in equation (37) to give a revised estimate of QAR(x +  $\Delta$ x). This new estimate then replaces the previous guess, and the entire procedure is repeated until successive values of QAR(x +  $\Delta$ x) do not differ appreciably.

The initial estimate of QAR(x +  $\Delta$ x) was obtained as follows. Substitut equation (36) in equation (37) for DQAR(x +  $\Delta$ x); solve the result for QAR(x +  $\Delta$ x) This leads to a first estimate as

$$QAR(x + \Delta x) = \frac{QAR(x) \left[1 - \varepsilon x \Delta x\right] + \frac{1}{2} \Delta x \left[DQA(x + \Delta x) + DQA(x)\right]}{1 + \varepsilon \Delta x (x + \Delta x)} - - - (53)$$

The values of DQA(x) and DQA( $\Delta x$ ) had already been computed as a step in the solution for QA, the amount absorbed, and were saved for use in this calculation.

The solution of equation (30) to obtain QAR for the constant base area model was accomplished in identical fashion (with the appropriate equations).

## (iv) Time for drop to disappear

This was computed for the constant radius of curvature and constant angle of contact models.

For the first case, consider equation (15), the analytic solution for drop height h ( $\equiv$ 2R-y) as a function of time. At the time t when the liquid drop has just disappeared, h=0, or y=2R. Then the value of x( $\equiv$  $\sqrt{t}$ ) which satisfies equation (15) for y=2R must be computed.

Substituting y=2R in equation (15) leads to

$$F(x) = \left[1 - \frac{x}{R} (C_2 + C_1 x)\right]^{\frac{1}{C_2}} (C_2^2 + 4C_1 R)^{\frac{1}{2}} - \left[1 - \frac{ho}{2R}\right]^{\frac{2}{C_2}} (C_2^2 + 4C_1 R)^{\frac{1}{2}}$$

$$\cdot \left[\frac{C_2}{2C_1 R} \left[(C_2^2 + 4C_1 R)^{\frac{1}{2}} - C_2\right] - 1\right] \left[\frac{2C_1 x + C_2 + (C_2^2 + 4C_1 R)^{\frac{1}{2}}}{2C_1 x + C_2 - (C_2^2 + 4C_1 R)^{\frac{1}{2}}}\right] = 0 - - - (54)$$

Since the initial drop size is used to compute R, all quantities in equation (39) except x are known. To solve for x, the Newton-Raphson formula is used iteratively. Let a first approximation to the root of equation (39) be  $\mathbf{x_n}$ ; then an improved value of the root,  $\mathbf{x_{n+1}}$ , is given by

$$x_{n+1} = x_n - \frac{F(x_n)}{F^1(x_n)}$$
 ---- (55)

where the function, F(x), and its derivative with respect to x,  $F^1(x)$ , are evaluated for  $x=x_n$ . This method converges quadratically to the correct root as repetitive iterations are performed.

If equation (39) is written symbolically, the evaluation of  $F^1(x)$  (and the numerical computation of  $x_{n+1}$ ) are more easily performed. That is, let

$$F(x) = (FA)^{\frac{FRT}{C_2}} - (FB)^{\frac{2FRT}{C_2}} [FC]^{\frac{FD}{FE}} - - - - - - - - - - - (56)$$

where FA, FRT, FB, FC, FD and FE are obvious when (41) and (39) are compared. Then

$$F^{1}(x) = -\frac{FRT}{C_{2}R} (FA)^{\frac{FRT}{C_{2}}} - 1 (C_{2} + 2C_{1}x) - (FB)^{\frac{2FRT}{C_{2}}} (FC)^{\frac{2C_{1}(FE - FD)}{(FE)^{2}}} - - - (57)$$

This is evaluated for each x=x and substituted in equation (40) until the required accuracy is obtained.

For the constant angle of contact model, consider equation (39b). At  $\tau$ , the instant of drop disappearance, h = 0;

then 
$$1 - m\tau - n\tau^{\frac{1}{2}} = 0$$

Hence 
$$\tau = \left[\frac{1}{2m} \left(-n \pm \sqrt{n^2 + 4m}\right)\right]^2$$
 ---- (58)

## POLYDISPERSE DROP DISTRIBUTION

It has been shown experimentally that the drop distribution from a spray tank or agricultural spray boom is well approximated by a Pearson distribution involving the Incomplete  $\Gamma$ -function (4).

The distribution function is given by

$$dN = KDe^{-bD^2}$$
  $dD - - - - - - - - - - - - - - (59)$ 

where dN = number of drops with diameters between D and D + dD,

K = constant

D = drop diameter

 $b=\frac{c}{\mu^2}$  , where  $\mu$  = mass median diameter and c = 2.1757.

Similarly, the mass of drops in this range is given by

Theoretically, either of these distribution functions can be combined with the previously derived differential equations of a single drop, to predict analytically the behaviour of the entire drop population. It has not been found possible to do this as yet for the constant radius of curvature model. In princi ple, this method can be used for the constant angle of contact model, but turns out to be impractical (See Appendix I). Instead, the distribution function has been approximated by a histogram, giving a series of drop sizes and appropriate weighting factors. The behaviour of a given size drop (as a function of time) was determined then at each time step required. The quantities calculated for all the drops of the histogram were weighted and added together to obtain values approximating those of the continuous distribution.

The calculation of the histogram drop sizes and weighting factors is straightforward. The mass distribution function is used. Let  $u = \sqrt{c} \frac{D}{\mu}$ ; then equation (44) becomes

where J = constant.

In the interval from  $D_1$  to  $D_2$ , the mass will be

$$M = J \int_{u_1}^{u_2} u^4 e^{-u^2} du$$

The total mass in the distribution will be

$$M_{T} = J \int_{0}^{\infty} u^{4} e^{-u^{2}} du$$

Hence the weighting factor for each histogram interval will be

$$\frac{M}{M_{T}} = \frac{\left[\frac{1}{2}ue^{-u^{2}} \left(u^{2} + 3/2\right) - \frac{3\sqrt{\pi}}{8} erf\left(u\right)\right]u_{1}^{2}}{\frac{3\sqrt{\pi}}{8}}$$

$$\frac{M}{M_{\rm T}} = \left[ \left( \frac{4}{3\sqrt{\pi}} u e^{-u^2} (u^2 + 3/2) - \text{erf (u)} \right) \right]_{u_1}^{u_2} - - - - - (62)$$

or

Now the centroid of each histogram interval will be given by

$$\overline{u} = \frac{u_1^{\int_{u_1}^{u_2} u dM}}{\int_{u_1^{u_2}}^{u_2} dM}$$

$$= \frac{\int_{u_{1}}^{u_{2}} u^{5}e^{-u^{2}}du}{\int_{u_{1}}^{u_{2}} u^{4}e^{-u^{2}}du}$$

Integration by parts leads finally to

$$\overline{u} = \sqrt{c} \frac{\overline{D}}{\mu} = \frac{\left[e^{-u^2} (u^4 + 2u^2 + 2)\right]_{u_1}^{u_2}}{\left[ue^{-u^2} (u^2 + 3/2) - \frac{3\sqrt{\pi}}{4} \operatorname{erf}(u)\right]_{u_1}^{u_2}} - - - - - - (63)$$

A computer program called HISTO has been written to compute histogram centroid values and weighting factors. The program calculates these values as a series of equal diameter intervals from 0 to 3 times the mass median diameter. This range will include more than 99% of the total mass in the continuous distribution. The computed values are punched out on data cards, and the cards subsequently used as input to polydisperse distribution programs. At present, 75 intervals are used in the histogram.

## RESULTS AND DISCUSSION

Using identical input parameters in each run, several comparison runs between analogue and digital monodisperse programs were made. The results agreed with each other at all times, usually to at least the third significant figure, thus verifying the self-consistency of the programs and the accuracy of the numer cal techniques of solution in the digital program.

Figure 2 shows a plot of pick-up versus time for monodisperse distribution, for both field experiments  $({}^7,8)$  and the digital computer results for the constant radius of curvature model. As previously discussed, the calculations were based on the assumption that constant meteorological conditions prevailed; ie, that  $C_1$ ,  $C_2$ , etc. are constants. This is an oversimplification which could easily be improved, for example, by replacing these constants with parameters which are functions of temperature, wind speed, and so on. The calculations would then be modified by the insertion as input to the program of actual meteorological observations, thus permitting the dependent meteorological parameters to be calculated for much shorter time intervals. However, the fit of theoretica points to experimental values, and to the general shape of the pick-up curve, is quite good without considering variations in meteorological effects.

A similar curve for evaporation, for the same distribution and model, is given in Figure 3. Again good agreement is obtained. However, as reported previously, the evaporative parameter required to produce approximately correct total evaporative amounts on prairie terrain is  $\sim$  5 times as great as that found in other experiments on smooth surfaces (9). There is some evidence that this increased value does indeed apply in this situation (10).

While experimental results for both pick-up and evaporation in the same experiment are scarce, Figure 4 shows a comparison between digital computer results for polydisperse and monodisperse distributions, using the constant radius of curvature model, and with the mass median diameter and all other parameters identical. The polydisperse curves show the expected rounding effects due to the range of drop diameters.

Both the analogue and digital monodisperse programs were modified to calculate the results for the constant base area model. A typical plot of results is shown in Figure 5. The evaporation curve is almost identical with that predicted by the constant area disc model (1,2). This is to be expected from Equation (25), where  $\frac{dQ_E}{dt} \propto (a^2+h^2)$ , since a, the base radius of the liquid drop, is approximately 10 times as large as h; consequently  $\frac{h^2}{a^2} \approx 1\%$ . Furthermore h is decreasing with time, thus  $Q_E \approx \text{const.} \times \text{time}$ , as the graph indicates. Figure 3, on the other hand, shows that the experimental evaporation curve is not of this form.

The constant angle of contact model produces curves which are similar to those of the constant radius of curvature model, as shown in Figure 6. These curves are perhaps somewhat more rounded than those of the latter model, but the differences are not great, and adjustment of the system parameter values can produce a close match of the two model predictions.

#### CONCLUSIONS

Three models of drop behaviour have been developed and solved by computer methods; the constant base area model, the constant radius of curvature model, and the constant angle of contact model. The models are based on the idealized case of discrete droplets on a smooth plane surface, but do provide a good fit to values obtained for evaporation and absorption from drops on rough natural prairie terrain. Extension of the models to incorporate variations due to changing meteorological conditions is quite feasible, and is being pursued. All models provide for the variation of the surface area of the drop with time, but the constant base area model allows too little variation to provide a reasonable fit to evaporation data. Consequently, the preferable approach appears to be that of the constant radius of curvature or constant angle of contact models.

The first preferred approach leads to differential equations which are generally analytically insoluble or mathematically intractable. However, numerical solutions to the equations have been obtained and appear quite satisfactory. The theoretical predictions agree quite well, both qualitatively and quantitatively, with the somewhat scarce experimental data.

The constant angle of contact model leads to equations which are generally analytically soluble. The fit to experimental data appears to be comparable to that of the previous model if the parameters are suitably chosen. Insufficient experimental evidence is available as yet to indicate which model is more suitable.

All models are directly applicable to calculation of behaviour of monodisperse distributions, but recourse to some numerical method of treating polydisperse drop distributions may be necessary. One approach, involving a histogram approximation to the continuous curve, is illustrated in this report for a Pearson Incomplete I-function distribution; this technique may be applied to any polydisperse distribution if the functional expression for drop size or mass versus diameter is known.

The decision in favour of either of the two best models, determinations of variations in absorptive and evaporative parameters with wind speed, temperature and terrain, etc., are handicapped by the relatively small amount of experimental data. Experiments are underway to expand the amount of data available in an attempt to answer some of these queries.

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## LIST OF SYMBOLS

| a                            |   | radius of base of drop on substrate   |
|------------------------------|---|---|
| Ao                           | _ | initial base diameter of drop on substrate  |
| As                           | _ | free surface area of drop on substrate  |
| b                            | - | $(\exists c/\mu^2)$ parameter in distribution function  |
| В                            | - | $(\exists R/h \text{ or } (l-\cos\alpha)^{-1}) \text{ constant in constant angle of contact model}$ |
| С                            | - | constant in distribution function (=2.1757)   |
| C <sub>1</sub>               | _ | coefficient of evaporation  |
| C <sub>2</sub>               | _ | coefficient of absorption   |
| DQA<br>DQE                   | - | derivatives of ${\tt Q}_A$ and ${\tt Q}_E$ with respect to the independent variable                 |
| FA,FB,FC,<br>FD,FE,FRT       | - | shorthand notation for terms in analytic solution of time for drop to disappear                     |
| h                            | - | height at any time at centre of drop on substrate   |
| K                            | - | $\left(\frac{1}{r_0}\right)$ constant dependent on $\lambda$  |
| m                            | - | evaporative factor in constant angle of contact model   |
| M                            | - | mass of liquid drops  |
| n                            | - | absorptive term in constant angle of contact model  |
| N                            | - | number of liquid drops  |
| Q <sub>A</sub> ,QA           | - | amount of liquid absorbed   |
| $\mathtt{Q}_{\mathrm{E}}^{}$ | _ | amount of liquid evaporated   |
| Q <sub>AR</sub> ,QAR         | - | amount of liquid absorbed and remaining in the substrate  |
| ro                           | - | original free drop radius   |
| R                            | - | radius of curvature at any time of free surface of drop on substrate                                |

## SYMBOLS (Cont'd)

u - dimensionless distribution function parameter

$$\left( \equiv \sqrt{c} \frac{D}{\mu} \right)$$

V - volume of drop at any time

x - transformed independent variable ( $\equiv \sqrt{t}$ )

y - transformed dependent variable (≡2R-h)

 $\Delta x$  - incremental change in x

angle of contact between liquid and substrate

ε - decay rate constant of liquid in substrate

 $\lambda$  - ( $\equiv A_0/D$ ) spread factor

μ - mass median diameter of drop distribution

## APPENDIX I

## POLYDISPERSE DROP DISTRIBUTION -

## Constant Angle of Contact Model

At any time  $\tau$ , minimum drop size remaining will be given by  $D_{min}(\tau) = \frac{2}{K} h_o(\tau) = \frac{2}{K} (m\tau + n\sqrt{\tau})$ , where  $m = \frac{2BC_1}{3B-1}$  and  $n = \frac{2(2B-1) C_2}{3B-1}$ .

Put 
$$\frac{2m}{K} = M$$
;  $\frac{2n}{K} = N$ ; then

$$D_{\min}(\tau) = M + N \sqrt{\tau}$$
 ---- (64)

First consider evaporation. The total amount evaporated up to any time t will consist of two components; the amount contributed by all drops still existing at time t - ie, those with diameters  $D \geqslant D_{\min}$ ; and the amount contributed by drops which have already completely disappeared - ie, those with  $D < D_{\min}$ . The amount contributed by the latter group will be a function of the time it took each drop size to disappear, as well as the total time involved. Hence the evaporation may be written in two parts:

$$Q_{E}(t) = \int_{0}^{t} \int_{D_{min}(t)}^{\infty} \left[ \frac{dQ_{E}}{dt} \right] dMd\tau + \int_{0}^{t} \int_{0}^{D_{min}(\tau)} \left[ \frac{dQ_{E}}{d\tau} \right] dMd\tau - - - (65)$$

where  $\frac{dQ_E}{dt}$  = rate of evaporation of a drop of size D

dM = number of drops with masses between D and D+dD

Also  $D_{min}(t) = minimum drop size remaining at time t$ 

and  $D_{\min}(\tau)$  = minimum drop size remaining at time  $\tau$ ,

where τ < t

Since  $\frac{dQ_E}{dt}$  is given by (40), and dM by (60), in terms of diameter D and time t, in principle both integrals can be evaluated analytically. However, the effort involved in working out an analytic expression for  $Q_E$  as a function of time will be considerable, if possible at all. It was not considered worthwhile, since though an expression for  $Q_A(t)$  might be arrived at after an equally great amount of labour, the analytic expression for  $Q_{AR}$  will be even more difficult to resolve, and may be completely unobtainable at all.

Consequently, though analytic expressions for pick-up, evaporation and absorption as functions of time are theoretically obtainable, the laborious and

complex algebra involved makes the effort not worthwhile, both from the point of view of correctly obtaining the analytical formulae, and of the computer time required to evaluate the lengthy resultant expressions. It was therefore decided to apply the same methods as used previously, that is, to approximate the polydisperse distribution by a histogram and then to evaluate each drop size interval independently, followed by a final summation of all intervals.

### APPENDIX II

## COMPUTER PROGRAMS FOR THE CONSTANT RADIUS OF CURVATURE MODEL

Both analogue and digital programs were written to provide solutions to drop behaviour. An analogue program is useful for several reasons: it can be quickly prepared, is very easily debugged, and provides a simple method of testing the basic model and obtaining reasonable trial values of parameters. However, it is very time consuming on the computer and is not suitable for multiple runs or extensive tabular output generation. It is, however, also helpful as a check on the accuracy of the digital computations, particularly when, as in this problem, the digital solutions are obtained by a series of numerical approximations.

The analogue program is written for the Continuous System Modeling Program (CSMP), a digital analogue simulation language for the IBM 1130 computer. The program for the solution of drop height, evaporation and absorptive quantities, and pick-up, is shown as a block diagram in Figure 7. Configuration data and initial conditions and parameter data are shown in Figures 8 and 9.

Two digital programs were written to compute pick-up, evaporation and absorption versus time. The first program was used for monodisperse and the second for polydisperse drop distributions. The polydisperse case was treated by dividing the distribution function into a histogram of 75 intervals, and considering each interval as a collection of drops of the same size. Consequently the second program differs from the first only in arranging the appropriate sequence and weighting factors for considering 75 different drop sizes, and summing the results at each time.

The digital programs are written in FORTRAN II for the IBM 1130 computer. The flow charts for the monodisperse and polydisperse cases are shown in Figures 10 and 11 respectively. They use input data formats as shown in Table I. The two FORTRAN programs are given in Figures 12 and 13.

### TABLE I

## I INPUT DATA FOR MONODISPERSE DISTRIBUTION

### PROGRAM PKUP3

First Card

EF1, EF2 - Efficiency factors for (1) pickup of free liquid, and (2) expression and pickup of liquid in substrate.

Format 2F10.0

Second Card C1 - Evaporative coefficient

C2 - Absorptive coefficient

LAMDA - Spread factor

DIAO - Mass median diameter (microns)

EPS - Mean decay rate of liquid in substrate

 $(\min^{-1})$ 

DELT - Time increments (min)

N - Number of time increments

Format 6F10.0, I3

Third, Fourth, etc. Cards

For subsequent runs, same as second

card.

## II INPUT DATA FOR POLYDISPERSE DISTRIBUTION

#### PROGRAM POLY MODEL MARK 3

First 22 Cards

- (DIA(I), WF(I), I=1,75)

Format 7E11.5

These are interval diameter values and weighting factors obtained when the Pearson distribution function is approximated by a histogram; the cards are obtained as output from Program HISTO.

Twenty-third Card EF1, EF2 - Efficiency factors for (1) pickup of free liquid, and (2) expression and pickup of liquid in substrate. Format 2F10.0.

Twenty-fourth Card C1 - Evaporative coefficient

C2 - Absorptive coefficient

LAMDA - Spread factor

DIAM - Mass median diameter (microns) of distribu

tion

EPS - Mean decay rate of liquid in substrate

 $(\min^{-1})$ 

DELT - Time increments (min)

N - Number of time increments

Format 6F10.0, I3

Twenty-fifth, Twenty-sixth, etc, Cards

For subsequent runs, same as 24th card.

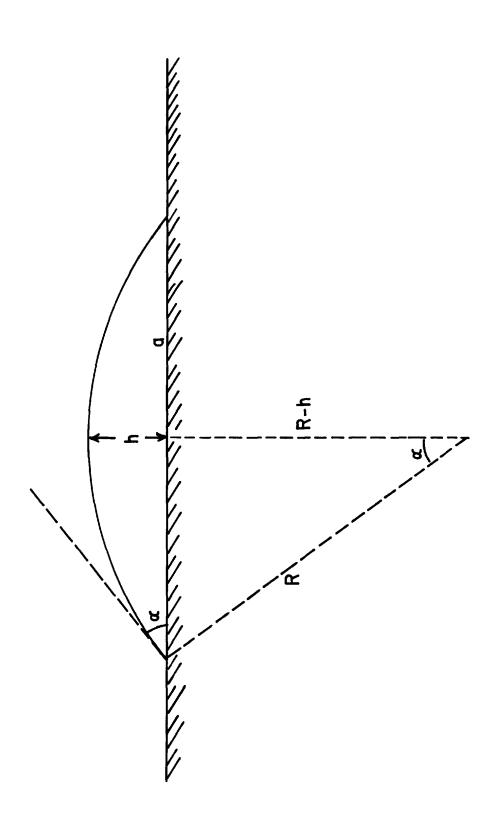
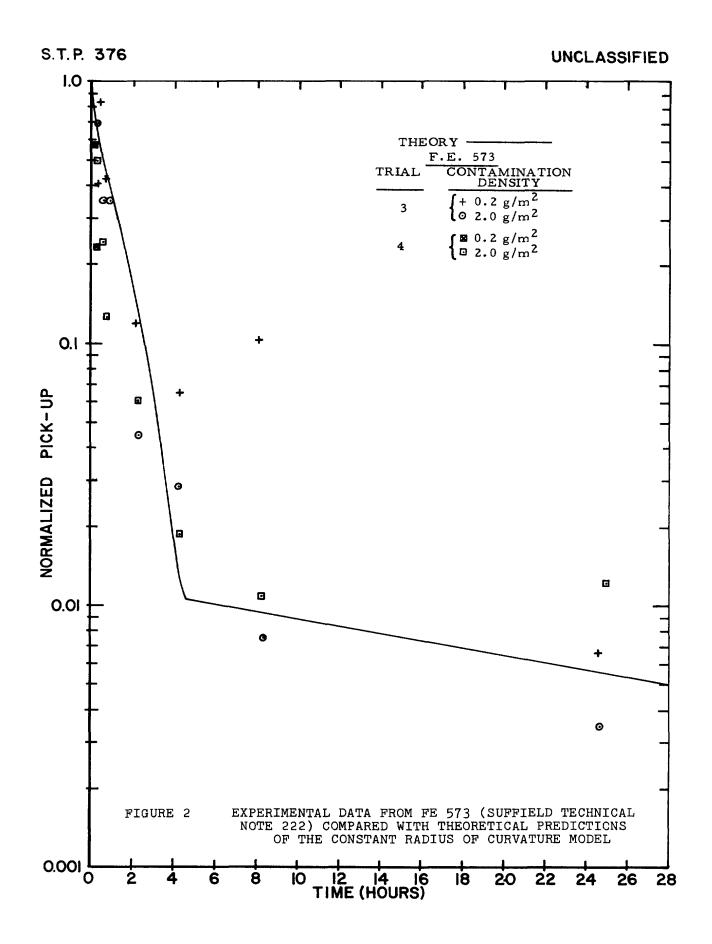
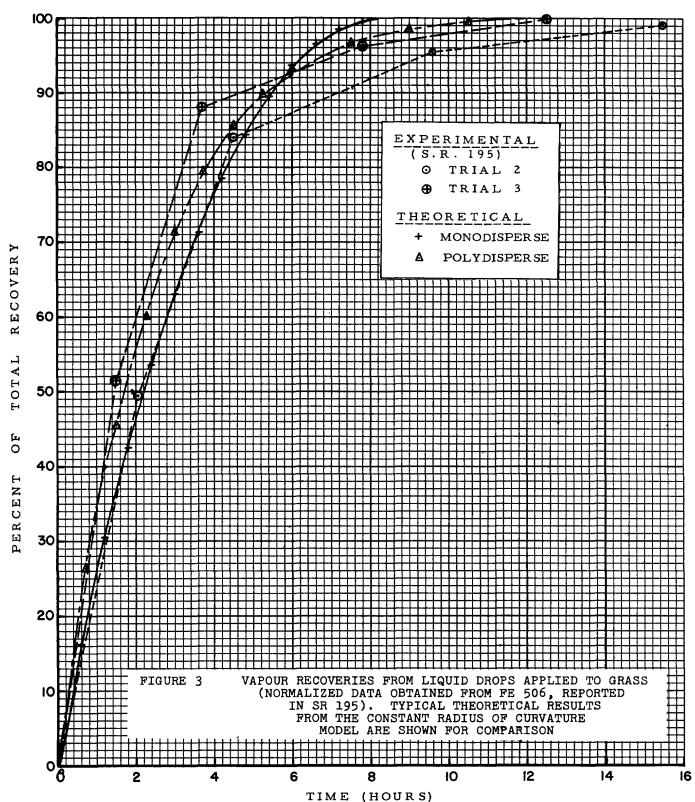
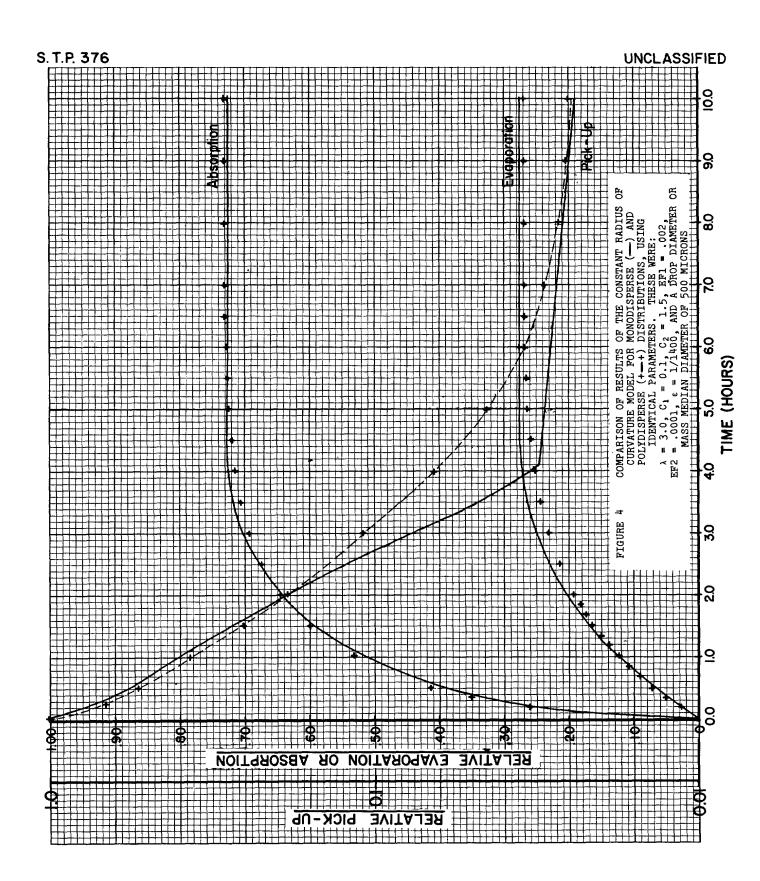


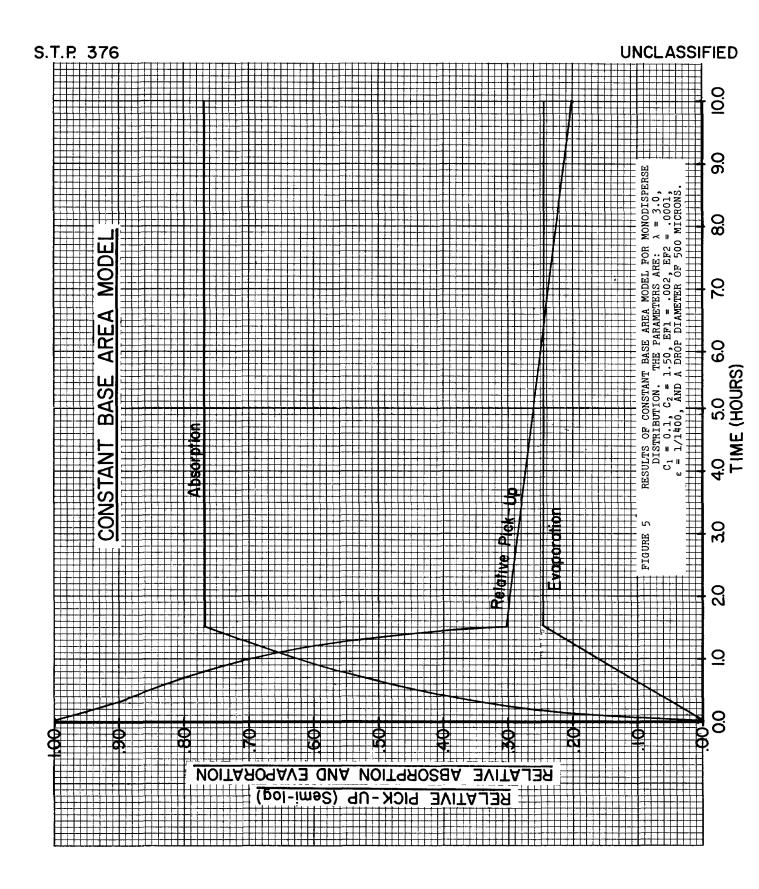
Fig. I General Varying Surface Area Model

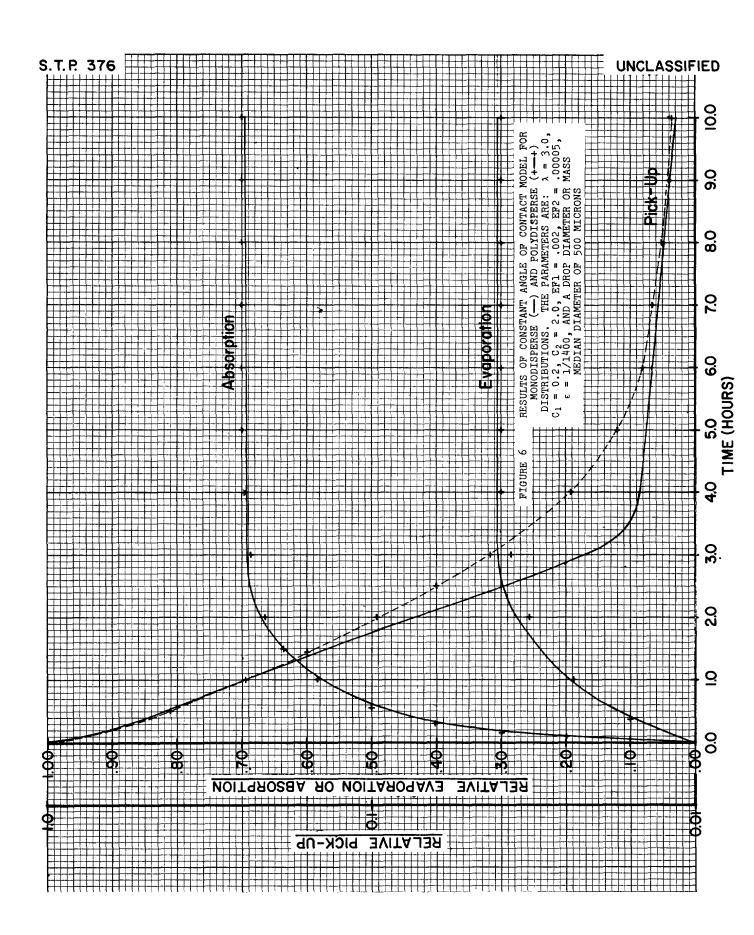


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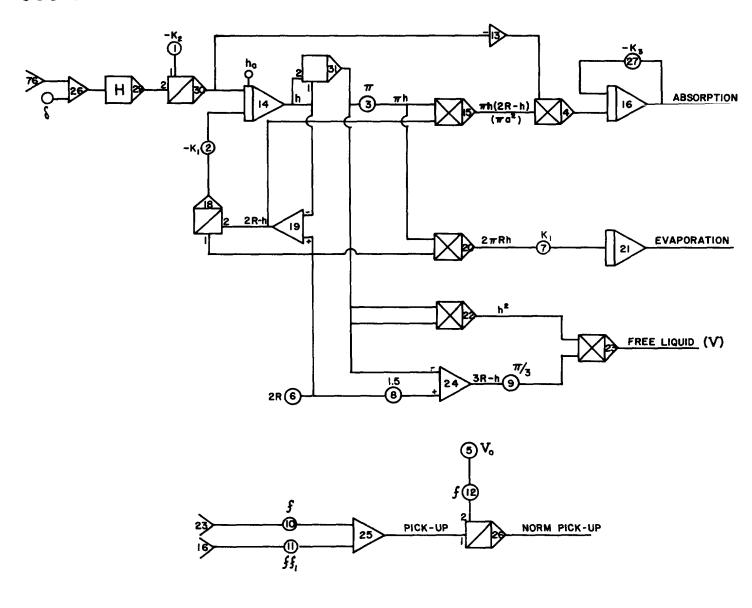






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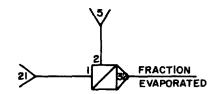


FIGURE 7 CSMP ANALOGUE DIAGRAM FOR CONSTANT RADIUS OF CURVATURE MODEL

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## CONFIGURATION SPECIFICATION

| OUTPUT NAME           | BLOCK    | TYPE   | INPUT 1 | INPUT 2 | INPUT 3 |
|-----------------------|----------|--------|---------|---------|---------|
| ABSORB. CONST.        | 1 2      | K      | 0       | O O     | 0       |
|                       | 2        | G      | 18      | 0<br>0  | 0       |
| -ARCORD BATE          |          | G      | 31      | •       | U       |
| -ABSORB. RATE<br>V(0) | 5        | X      | 15      | 13      | 0       |
| 2 R                   | 5<br>6   | K<br>K | 0       | 0<br>0  | 0       |
| -EVAP. RATE           | 7        | Ğ      | 20      | 0       |         |
| 3R                    | 8        | G      | 20<br>6 | 0       | 0       |
| 3 K                   | 9        | G      | 24      | Õ       | Ö       |
| LIQ. PICKUP           | 10       | Ğ      | 23      | Õ       | Ö       |
| SUB. PICKUP           | 11       | Ğ      | 16      | Õ       | ŏ       |
| PICKUP(0)             | 12       | Ğ      | 5       | ŏ       | ŏ       |
|                       | 13       | _      | 30      | Ō       | ā       |
| н                     | 14       | 1      | 30      | 2       | Ŏ       |
| BASE AREA             | 15       | X      | 3       | 19      | Ö       |
| TOTAL ABSORB.         | 16       | 1      | 27      | 4       | 0       |
|                       | 18       | 1      | 6       | 19      | Ó       |
|                       | 19       | +      | -14     | 6       | 0       |
| SURF. AREA            | 20       | X      | 3       | 6       | 0       |
| TOTAL EVAP.           | 21       | 1      | 7       | 0       | 0       |
|                       | 22       | X      | 31      | 31      | 0       |
| V                     | 23       | Χ      | 22      | 9       | 0       |
|                       | 24       | +      | -31     | 8       | 0       |
| PICKUP                | 25       | +      | 10      | 11      | 0       |
| NORM. PICKUP          | 26       | /      | 25      | 12      | 0       |
| SUB. DECAY CONS       | T 27     | G      | 16      | 0       | 0       |
| T + DELTA             | 28       | 0      | 76      | 0       | 0       |
|                       | 29       | Н      | 28      | 0       | 0       |
|                       | 30<br>31 | _      | .1      | 29      | 0       |
|                       |          | Ŕ      | 14      | 14      | 0       |
|                       | 32       | /      | 21      | 5       | 0       |

FIGURE 8 CONFIGURATION SPECIFICATIONS FOR CSMP PROGRAM

# INITIAL CONDITIONS AND PARAMETERS

| IC/PAR NAME | BLOCK | IC/PAR1      | PAR2     | PAR3     |
|-------------|-------|--------------|----------|----------|
| -K2         | 1     | -1.000000    | 0.00000  | 0.000000 |
| -K1         | 2     | -0.010000    | 0.000000 | 0.000000 |
| PI          | 3     | 3.141592     | 0.000000 | 0.000000 |
| V(0)        | 56541 | +9848.109375 | 0.000000 | 0.000000 |
| 2 R         | 6     | 7694.300792  | 0.000000 | 0.000000 |
| K1          | 7     | 0.010000     | 0.000000 | 0.000000 |
|             | 8     | 1.500000     | 0.000000 | 0.000000 |
| P1/3        | 9     | 1.047197     | 0.00000  | 0.000000 |
| F           | 10    | 0.002000     | 0.000000 | 0.000000 |
| F*F1        | 11    | 0.000100     | 0.000000 | 0.000000 |
| F           | 12    | 0.002000     | 0.000000 | 0.000000 |
| H(0)        | 14    | 73.825012    | 1.000000 | 0.000000 |
|             | 16    | 0.000000     | 1.000000 | 0.000000 |
| -K3         | 27    | -0.000714    | 0.000000 | 0.000000 |
| DELTA       | 28    | 0.010000     | 0.000000 | 0.000000 |

FIGURE 9 INITIAL CONDITIONS AND PARAMETERS FOR TYPICAL RUN OF CSMP PROGRAM

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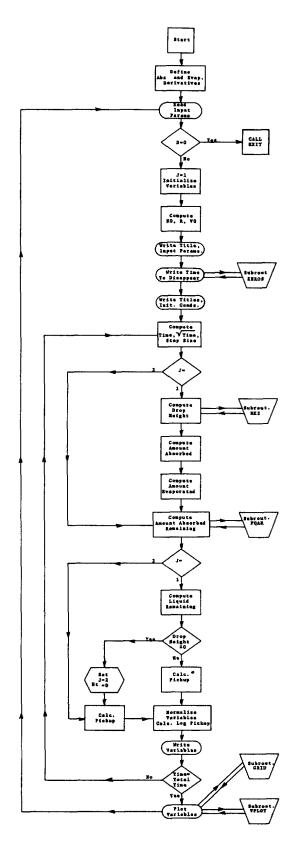


FIGURE 16: MCHODISPERSE FICKUP MODEL MARE )

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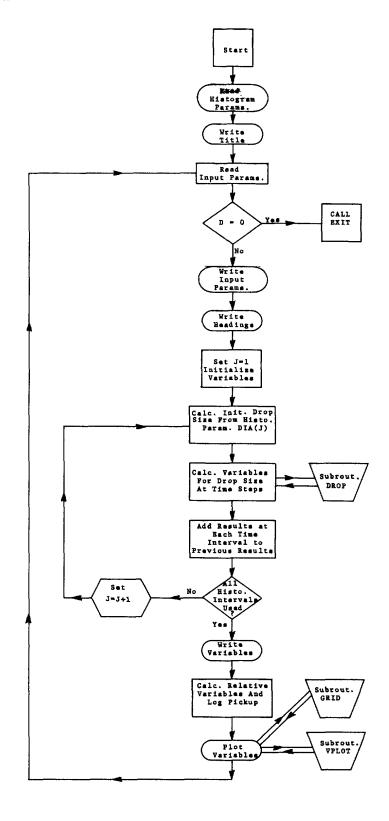


FIGURE 11(a): POLYDISPERSE PICKUP MODEL MARK 3

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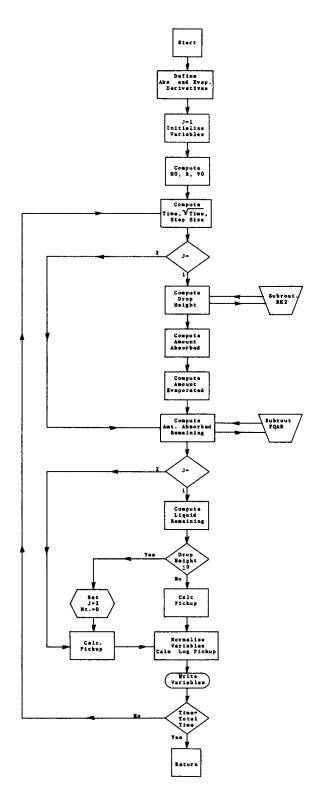


FIGURE 11(b): SUBROUTINE DROP

```
S T.P 376
                                                                                                                                                                                                                                                                                                                                        UNCLASSIFIED
            // JOB T
// FOR
ONE WORD INTEGERS
EXTENDED PRECISION
SUBROUTINE RK2 (FUN.H.XI.YI.K.N.YEC)
C RUNGE-KUTTA METHOD
DIMENSION VEC (1)
                                                                                                                                                                                                                                                                                                      RK2
                                                                                                                                                                                                                                                                                                                                 1
                                   DIMENSION VEC (1)
H2-H/2.
Y=YI
X=XI
DO 2 I-1.N
DO 1 J-1.K
T1-MFUN (X-Y)
T2-MFUN (X-H2-Y6T1/2.)
T3-MFUN (X-H2-Y6T2/2.)
T4-MFUN (X-H2-Y6T2/2.)
Y- Y6 (T162.*T262.*T36T4) /6.
X:XEM
                                                                                                                                                                                                                                                                                                       RK2
                                                                                                                                                                                                                                                                                                      RK2
RK2
RK2
RK2
                                    X=X6H
VEC (I) = Y
RETURN
END
           CALL EGRID(3+0+1+1+10)
A = 0.
D = 1 1 = 1+1
CALL ECHAR(-20+A,-+04+13++3+0+)
AP = A/60.
WRITE (7+50) AP
50 FORMAT (F4-1)
51 A = A + 60+00001
A = 0.
D = 22 1 = 1+11
CALL ECHAR(-36++(A-+015)++1++3+0+)
WRITE (7+53) A
53 FORMAT(F4-2)
54 A = A + +100001
            52 A = A + .100001
RETURN
END
// DUP
        COMMON C1.C2.R.DGAO.DGA4.XI.H.EPS.

1VTIME(100)

M = N + 1

CALL EPLOT(-2.VTIME(1).VQA(1))

DO 1 | = 2.M

1 CALL EPLOT(0.VTIME(1).VQA(1))

CALL EPLOT(-2.VTIME(1).VQE(1))

CALL EPLOT(-2.VTIME(1).VQE(1))

CALL EPLOT(0.VTIME(1).VQE(1))

CALL EPLOT(1.YTIME(1).RPKPL(1))

CALL EPLOT(1.YTIME(1).RPKPL(1))

DO 3 | = 2.M

3 CALL EPLOT(0.VTIME(1).RPKPL(1))

CALL EPLOT(1.YTIME(1).RPKPL(1))

CALL EPLOT(0.VTIME(1).RPKPL(1))

CALL EPLOT(0.VTIME(1).RPKPL(1))

CALL EPLOT(+1.720..0.)

RETURN

END

// DUP

**STORE WS UA VPLOT

// FOR

**ONE WORD INTEGERS

** EXTENDED PRECISION

FUNCTION FUNY(X,Y)

C USED BY RUNGE-KUTTA SUBROUTINE

COMMON C1.C2.R.DGAO.DGA4.XI.+H.EPS

FUNY = 4.*R**C1**X/Y + 2.*C2

RETURN

END
                                     RETURN
END
             // DUP
                                                           WS UA FUNY
            *STORE WS UA FURY
// FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION
SUBROUTINE ZEROS(HO)
COMPUTES TIME FOR DROP TO DISAPPEAR
COMMON C1+C2+R
                             x = 10.

RTF = SQRT(C2+#2 + 4.0+R*C1)

FB = (1.-.5+HO/R)+#(2.0+RTF/C2)

FC = 1.-.5+C2+(RTF-C2)/(R*C1)

1 FA = 1.-X#(C2+C1*X)/R
```

FIGURE 12 FORTRAN II PROGRAM FOR CONSTANT RADIUS OF CURVATURE MODEL AND FOR MONODISPERSE DISTRIBUTIONS. FOR COMPUTING DROP SIZE VS TIME, EITHER OF THE SUBROUTINES RK2 OR FNEWT MAY BE USED IF THE FORMER, THEN IN THE MAIN PROGRAM, STATEMENT NUMBER 9 BECOMES: 9 CALL RK2 (FUNY, H, TIME 1, Y14, 3, 4, VEC)

```
FD = RTF + C2 + 2.*C1*X
FE = 2.*RTF - FD
FX = FA**(RTF/C2) - FB**FC**FD/FE
DFX = ((C2+2.*C1*X)*RTF/(R**C2))*(FA**(RTF/C2-1.*))+FB**FC**4.**C1**
1RTF/(FE**2)
X1 = X + FX/DFX
1F (ABS(X1/X - 1.*) - *001)12*12*3
3 X = X1
50 Y0 1
               GO TO 1
12 TSO = X1==2
WRITE (3+4) TSO
4 FORMAT(6X, DROP DISAPPEARS AT', F8.3+1X, MINUTES', //)
  c
                            RETURN
END
 END
// DUP

*STORE WS UA ZEROS
// FOR
ONF WORD INTEGERS

* FXTENDED PRECISION
SUBROUTINE FNEWT(YI4.TIME1.HO.VEC)
COMPUTES DROP HEIGHTS BY NEWTON-RAPHSON METHOD
DIMENSION.VEC(4)
COMMON C1.C2.R.DQAO.DQA4.XI.H
  c
                            YO = 2.*R - HO
Y = Y14
X = TIME1
RTF = SQRT.(C2**2 + 4.*R*C1)
FC = .5*C2*(RTF - C2)/(R*C1) = 1.
  c
  c

1 FA =(Y$#2 - 2.*C2*X*Y - 4.*R*C1*X**2)/(YO**2)
FAP = FA**(RTF/C2)
FD = 4.*R*C1*X + Y**(C2 + RTF)
FE = 4.*R*C1*X + Y**(C2 - RTF)
FY = FAP - FC**(FD/FE)
DFY = 2.*R*TF**(Y**C2*X)*FAP/(C2*FA*YO**2)*FC**8.*R**C1*X*RTF/(FE**2)
YNEW = Y - FY/DFY

IF (ABS(YNEW/Y - 1.*) - .000001) 2.*2.*3
                    3 Y - YNEW
GO TO 1
  c
                   2 VEC(1) = YNEW
                            RETURN
END
RETURN

// DUP

>STORE WS UA FNEWT

// FOR

**ONE WORD INTEGERS

**EXTENDED PRECISION

FUNCTION FORRECTOR TO ADVANCE GAR BY H

COMMON (1.c2.R.DQAO.DOA4.XI.H.EPS

QAR3 = (DAR1+(1.=12.#H*EPS*XI) + ($.*H)*(DQA4+DQA0])/(1.*12.*

IHMEPS*(XI + 12.*H)

DOAR1 = DOAO -2.*XI*EPS*CAR1

3 DOAR3 = DOAO -2.*XI*EPS*(XI + 12.*H)*OAR3

FGAR = QAR1 + 6.*H*(DQAR3 + DQAR1)

IF (ABSIFGAR/QARS = 1.) - .0001) 1.*1.*2

2 QAR3 = EQAR

GO TO 3

1 RETURN

END

// DUP

**STORE WS UA FQAR

// FOR
 ## STORE ## S UA FGAR

*/ FOR

#ONE WORD INTFGERS

*10CS(CARD)

*10CS(1132 PRINTER)

* 10CS(PLOTTER)

* 10CS(PLOTTER)

* EXTENDED PRECISION

C PROGRAM PKUP3

REAL LAMDA,K1.*K2

EXTERNAL FUNY

DIMENSION VEC(4)

COMMON C1,C2-R.*DOAO.*DOA4.*X1.*H.*EPS.*VGA(100).*VGE(100).*RPKPL(100).*

1VTIME(100)

OPFINED PRIVATIVES OF MASS ARS. AND EVAP. TERMS
LOMBOUR C1,5C2-R.DQAG.DQA4.X].H.EPS.VQA(100).VQ

1VTIME(100)

C DEFINE DERIVATIVES OF MASS ABS. AND EVAP. TERMS

FNA(Y) = 2.0P10C204V-(2.0R-Y)/VO

FNE(X:Y) = 4.0P10C104R0X-(2.0R-Y)/VO

PI = 3.141992654

C READ INPUT PARAMETERS

22 READ (2.33) EF1.0EF2

33 FORMAT (2F10.0)

IF (EF1) 23.23.24

24 READ (2.2) C1:C2.LAMDA.DIAO.EPS.DELT,N

2 FORMAT (6F10.00.13)

C DEFINE INITIAL CONDITIONS

TIME = 0.

VTIME(1) = 0.
```

FIGURE 12
(Cont'd)
FORTRAN II PROGRAM FOR CONSTANT RADIUS OF CURVATURE MODEL
AND FOR MONODISPERSE DISTRIBUTIONS. FOR COMPUTING DROP SIZE
VS. TIME, EITHER OF THE SUBROUTINES RK2 OF FNEWT MAY BE USED.
IF THE FORMER, THEN IN THE MAIN PROGRAM, STATEMENT NUMBER
9 BECOMES 9 CALL RK2(FUNY, H, TIME 1, YI4, 3, 4, VEC)

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OA1 = 0.
 VOA(1) = 0.
 OE[ = 0.
 VOE(1) = 0.
 OE[ = 0.
 VOE(1) = 0.
 OED = 0.
 TIME1 = 0.
 REKUP = 1.
 REK C DO 1 I = 1.N
C DETERMINE STEP SIZE
TIME = TIME + DELT
VTIME(I+1) = TIME
TIME2 = SORT(TIME)
XI = TIME2
H = (TIME2 - TIME1)/12.
GO TO (9.10).J
CALCULATE OROP MEIGHT AT NEXT TIME INTERVAL 9 CALL FNEWT(YI4.TIME1.HO.VEC) YII = VEC(1) YI2 = VEC(2) YI3 = VEC(3) YI4 = VEC(4) // XEQ FORTRAN II PROGRAM FOR CONSTANT RADIUS OF CURVATURE MODEL AND FOR MONODISPERSE DISTRIBUTIONS. FOR COMPUTING DROP SIZE VS TIME, EITHER OF THE SUBROUTINES RK2 OR FNEWT MAY BE USED. IF THE FORMER, THEN IN THE MAIN PROGRAM, STATEMENT NUMBER 9 BECOMES 9 CALL RK2(FUNY, H, TIME 1, YI4, 3, 4, VEC)

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                                                                                                                                                                                                                                                                                                                                                                                                                                   UNCLASSIFIED
     // ZOR
   // JOS ...

*ONE WORD INTEGERS

* EXTENDED PRECISION

SUBROUTINE RK2 (FUN. H. XI. YI. K. N. VEC)

CHARLETTA METHOD
                                                                                                                                                                                                                                                                                                                                                                              RK2
                                                                                                                                                                                                                                                                                                                                                                                                                1
                         RUNGE-KUTTA METHOD
DIMENSION VEC (1)
HZ+H/2.
                              H2*H/2.
Y*YI
X XI
DO 2 I*1.N
DO 1 J*1.K
T1.*H*FUN (X6,Y)
T2*H*FUN (X6H2.*Y6T1/2.)
T3*H*FUN (X6H2.*Y6T2/2.)
T4*H*FUN (X6H2.*Y6T3)
Y * Y6 (T162.*T262.*T36T4) /6.
X*X6H
END
END
                                                                                                                                                                                                                                                                                                                                                                              RK2
                                                                                                                                                                                                                                                                                                                                                                                                           16
    // DUP
                                                                 WS UA RK2
   #STORE WS UA RK2

// FOR

**ONE WORD INTEGERS

** FXTENDED PRECISION

SUBROUTINE GRID

C PLOTTER FRAME AND SCALES

CALL SCALE(.01666667,10.,0.,0.)

CALL EGRID(0,0.,0.,60.,10)

CALL EGRID(1,600.,0.,10)

CALL EGRID(2,600.,1.,60.,10)

CALL EGRID(3,0.,1.,1.)
                    A.= 0.

00 51 I = 1.11

CALL ECHAR(-20.+A,-.04,.13..3.0.)

AP = A/60.

WRITE (7.50) AP

50 FORMAT (F4.1)

51 A = A + 60.00001

A = 0.

00 52 I = 1.11

CALL ECHAR(-36..(A-.015)..1..3.0.)

WRITE (7.53) A

53 FORMAT(F4.2)
                                 A = A + .100001
RETURN
                                     END
    *STORE WS UA
// FOR
*ONE WORD INTEGERS
                                                                 WS UA GRID
    # EXTENDED PRECISION
SUBROUTINE VPLOT
C DRAWS PLOTS
                      SUBROUTINE VPLOI

DRAWS PLOTS

REAL LAMDA

COMMON C1 oc2*LAMDA*DIAO*EPS*N*R*DQAO*DQAA*XI*H*VQA(61)*VQE(61)*

IPKUP(61)*VQAR(61)* VTIME(61)*PQAT(61)*PQET(61)*RPKPL(61)

M = N + 1

CALL EPLOT(-2*VTIME(1)*PQAT(1))

CALL EPLOT(-0*VTIME(1)*PQET(1))

CALL EPLOT(-2*VTIME(1)*PQET(1))

CALL EPLOT(-2*VTIME(1)*PQET(1))

DO 2 I = 2*M

2 CALL EPLOT(0*VTIME(1)*PQET(1))

CALL EPLOT(0*VTIME(1)*PRFPL(1))

CALL EPLOT(-2*VTIME(1)*PRFPL(1))

CALL EPLOT(-2*VTIME(1)*RPKPL(1))

DO 3 I = 2*M

3 CALL EPLOT(0*VTIME(1)*RPKPL(1))

CALL EPLOT(0*VTIME(1)*RPKPL(1))

CALL EPLOT(-2*VTIME(1)*RPKPL(1))

CALL EPLOT(-2*VTIME(1)*RPKPL(1))
                                    END
      // DUP
                                                                 WS UM VPLOT
      // FOR
   // FOR
*ONE WORD INTEGERS
* EXTENDED PRECISION

FUNCTION FUNY(X**)

C USED BY RUNGE-KUTTA SUBROUTINE

REAL LAMDA

COMMON C1**C2**LAMDA**DIAO**EPS**N**R**DQAO**DQA4**XI**H

FUNY = 4**R**C1**X/Y + 2**C2

PETIEN
                                    RETURN
      // DUP
     #STORE WS UA
// FOR
#ONE WORD INTEGERS
                                                                 WS UA FUNY
    **EXTENDED PRECISION

FUNCTION FOAR(GAR1)

C PREDICTOR-CORRECTOR TO ADVANCE GAR BY H

REAL LAMDA

COMMON C1:C2+LAMDA:DIAO:EPS:N:R:DQAO:DQA4:XI:H

QAR3 = (QAR1*(1--12:*H*EPS*XI) + (6:*H)*(DQA4+DQAO)}/(1:+12:*
                                1H#EPS#(XI + 12.#H))
DQAR1 = DQAO -2.#XI#EPS#QAR1
```

```
*STORE
            WS UA DROP
// FOR
*ONE WORD INTEGERS
#IOCS(CARD)
#IOCS(1132 PRINTER)
* IOCS (PLOTTER)
* EXTENDED PRECISION
   POLY MODEL MARK 3 , 20 FEB 1970
      REAL LAMDA
      DIMENSION DIA(75) + WF(75) + PQART(61) + RPKPT(61)
      COMMON C1.C2.LAMDA.DIAO.EPS.N.R.DQAO.DQA4.XI.H.VQA(61).VQE(61).
     1RPKUP(61), VQAR(61), VTIME(61), PQAT(61), PQET(61), RPKPL(61)
      READ (2+11) (DIA(1)+WF(1)+1=1+75)
   11 FORMAT (7E11.5)
      WRITE (3.1)
    1 FORMAT(1H1,15%, POLYDISPERSED MODEL MARK 3, 20 FEB 1970',/}
   10 READ (2.2) C1.C2.LAMDA.DIAM.EPS.DELT.N
    2 FORMAT(6F10.0:13)
      IF (DIAM) 23,23,24
   24 WRITE (3.3) LAMDA, DIAM, C1, C2, EPS
    3 FORMAT(/+5X+'LAMBDA = 1+F5+2+3X+'MMD ='+F7+2+1X+'MICRONS'+/+5X+
     1'C1 = '*F7*3*3X*
     1'C2 = '.F6.2.3X. 'EPSILON = '.F10.8.//)
      WRITE (3.4)
    4 FORMAT(5X, TIME, 4X,
                                      'AMT. ABS.',3X,'AMT. EVAP.',4X,
     1'AMT. ABS.',4X, 'REL',/,4X, '(MINS)',
                                                        4X. PERCENT'.5X.
     2'PERCENT', 6X, 'REMAINING', 3X, 'PICKUP',/)
C SET STARTING CONDITIONS
      N1 = N + 1
      DO 6 I = 1.N1
      RPKPT(I) = 0.
      PQAT(I) = 0.
      PQET(I) = 0.
      PQART(1) = 0.
      VTIME(1) = DELT + FLOAT(1-1)
      DO 5 J = 1:75
DIAO = DIA(J) * DIAM
      CALL DROP
      DO 5 I = 1.N1
      RPKPT(I) = RPKPT(I) + RPKUP(I)*WF(J)
      PQAT(I) = PQAT(I) + VQA(I) + WF(J) +100.
      PQET(1) = PQET(1) + VQE(1) + WF(J) +100.
    5 PQART(I) = PQART(I) + VQAR(I)*WF(J)*100
      WRITE(3,7)(VTIME(I),PQAT(I),PQET(I),PQART(I),RPKPT(I),I=1,N1)
    7 FORMAT (4X, F6.1, 1X, F10.2, 2X, F10.2, 2X, F10.2, 6X, F6.4)
      DO 15 I = 1:N1
      PQAT(I) = PQAT(I)/100.
      PQET(1) = PQET(1)/100.
   15 RPKPL(I) = .217147#ALOG(RPKPT(I)) + 1.
      CALL GRID
CALL VPLOT
      GO TO 10
   23 CALL EXIT
      END
// XEQ
// PAUS
```

```
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                                                                                                                                                                                                                                                                                                                                                 UNCLASSIFIED
         3 DQAR3 = DQA4 - 2.*EPS*(XI + 12.*H)*QAR3
FGAR = QAR1 + 6.*H*(DQAR3 + DQAR1)
1F (ABS(FGAR/QAR3 - 1.) - .0001) 1.1.2
2 QAR3 = FGAR
GO TO 3

1 RETURN
END
// DUP
**STORE WS UA FQAR
      #STORE WS UA FQAR

// FOR

#ONE WORD INTEGERS

# EXTENDED PRECISION
SUBROUTINE DROP

O ETERMINES BEMAVIOUR OF DROP OF GIVEN SIZE

RFAL LAMDA K1 * K2

EXTERNAL FUNY

DIMENSION VEC(4)

COMMON C1 * C2 * LAMDA * DIAO * EPS * N * R * DQAO * DQA 4 * XI * H * VQA (61) * VQE (61) *

1 RPUP(61) * VQAR(61) * VTIME(61) * PQAT(61) * PQET(61) * RPKPL(61)

C DEFINE DERIVATIVES OF MASS ARS * AND EVAP * TERMS

FNA(Y) = 2 * PPI * PC * 2 * P * PC * 2 * P * PC * Y * VO

FNE(X * Y) = 4 * * PPI * C1 * PR * X * Y * VO

PI = 3 * 141392654
      FNA(Y) = 2.*PI#C2*Y*(2.*R-Y)/VO

FNE(X,Y) = 4.*PI#C1*R*X*(2.*R-Y)/VO

PI = 3.41.592654

C SET STARTING CONDITIONS

J = 1

OA1 = 0.

VOA(1) = 0.

OE1 = 0.

VOA(1) = 0.

OAR1 = 0.

VOA(1) = 0.

OAR1 = 0.

VOA(1) = 0.

DOE0 = 0.

TIME1 = 0.

RPKUP(1) = 1.

COMPUTE HOLR AND VO

K1 = SORT(16.+LAMDA**6)

K2 = (4.*K1)**(1./3.) - (K1-4.)**(1./3.)

HO = K2*RO

R = ((4.*K2*R3)/(3.*K2**2))**RO

VO = (4.*K2*R3)/(3.*K2**2))**RO

VO = (4.*K2*R3)/(3.*K2**2))**RO

VO = (4.*K2*R3)/(3.*K2**2))**RO

VO = (4.*K2*R3)/(3.*K2**2))**RO

VO = (4.*K2*R3)/(3.*K2*R3)/(3.*K2*R3))**AD

HITE = HO

DOA0 = FNA/V14)
                                Y14 = 2. #R - HO
DQA0 = FNA(Y14)
         - DO 1 1 . 1.N
      TIME: TIME: VQAR(I+1) = QAR1
VQA(I+1) = QAR1
VQE(I+1) = QE1
1 RPKUP(I+1) = PKUP/*002
       RPKUP()
RETURN
END
// DUP
```

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This paper continues the development of physical and mathematical models applicable to liquid drop absorption and evaporation from a substrate. Three examples are considered: a constant radius of curvature model; a constant base area model; and a constant angle of contact model. All allow the free surface area of the drop to vary with time. Methods of solution are given for both monodisperse and polydisperse drop distributions, and the results are compared with experimental data. Both the constant radius of curvature and constant angle of contact versions provide reasonable fits to experiment.

#### Security Classification

#### KEY WORDS

- 1. Mathematical Models
- Physical Models
- 3. Drop Absorption
- 4. Drop Evaporation
- 5. Vapour Evolution
- 6. Pick-up Hazard

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