AD-772 539

AN ANALYTICAL AND COMPUTATIONAL MODEL OF THE GROWTH OF WATER AND ICE PARTICLES IN NUCLEAR-EXPLOSION CLOUDS

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Prepared for:

Defense Nuclear Agency

24 December 1973

AD 772 539

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS
BEFORE COMPLETING FORM

1. REPORT NUMBER DNA 3173F	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) An Analytical and Computational Model of the Growth of Water and Ice Particles in Nuclear-Explosion Clouds		5. TYPE OF REPORT & PERIOD COVERED Final Report
		6. PERFORMING ORG. REPORT NUMBER ERG F-73-1
7. AUTHOR(s) Heubsch, Ian O.		8. CONTRACT OR GRANT NUMBER(s) DNA001-72-C-0121
9. PERFORMING ORGANIZATION NAME AND ADDRESS Euclid Research Group 1760 Solano Avenue Berkeley, California 94707		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS NWED Code A Task and Subtask Code A127 Work Unit Code 40
11. CONTROLLING OFFICE NAME AND ADDRESS Defense Nuclear Agency Washington, D.C. 20305		12. REPORT DATE December 24, 1973
		13. NUMBER OF PAGES 57
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

This work was supported by the Defense Nuclear Agency under Subtask AA127-40.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Nuclear weapons effects; computational models; aerosols; particle formation; condensation; agglomeration.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report describes development of the AEROSOL program for modeling growth of water and ice particles in nuclear-explosion clouds. AEROSOL has been developed for incorporation into an expanded version of the SHELL hydrocode which describes the evolution of the nuclear cloud environment. The report summarizes the physics, mathematical formulation, and particle-size classification scheme used in the program. It includes a listing of the AEROSOL program and recommendations for further program development.

SUMMARY

This report describes development of the AEROSOL program for modeling growth of water and ice particles in nuclear-explosion clouds. AEROSOL has been developed for incorporation into an expanded version of the SHELL hydrocode which describes the evolution of the nuclear cloud environment. The report summarizes the physics, mathematical formulation, and particle-size classification scheme used in the program. It includes a listing of the AEROSOL program and recommendations for further program development.

CONTENTS

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SECTION 1
INTRODUCTION, BACKGROUND, AND OBJECTIVE

1.1 NUCLEAR CLOUD PHENOMENA AND HAZARDS

The fireball produced by an atmospheric nuclear explosion rises as a buoyant nuclear cloud, which stabilizes near its maximum altitude, continues to expand and diffuse, and eventually dissipates. Associated with the cloud development are physical phenomena including ionization of the air, intense turbulence, and formation and dispersion of cloud debris, including radioactive fallout particles. The cloud contains water vapor, whose potential sources are entrained atmospheric moisture, and also, if the explosion occurs near the sea or land surface, sea water or ground water. As the cloud rises, entrains air, expands and cools, much of the water vapor condenses into water and ice. The water-substance particles continue to grow by condensation and agglomeration. Besides water, the particles may contain debris from the nuclear device, and dust (i.e., soil and rock materials) or sea salt, in amounts depending on the burst location.

The nuclear cloud and its particulate contents present potential hazards, including:

1. Mechanical damage to missiles and aircraft passing through the cloud.
2. Degradation or blackout of communications and reconnaissance systems.
3. Radiation from fission products and other radionuclides.

The extent of each of these hazards depends on the mass-concentration and particle-size distribution of the nuclear cloud particles.

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1.2 COMPUTATIONAL CLOUD MODELS

Analytical models of nuclear-cloud development have been developed to predict and estimate the magnitude of the hazards mentioned above. As with all theoretical models, it is desirable to compare the predictions with experimental data. Actual data available from nuclear-explosion tests are highly scattered, incomplete and uncertain. Useful types of data include photographic and radar observations of nuclear clouds, and samples of particle mass and radioactivity from airborne and ground collectors. Radar observations are especially important for checking cloud models that consider the cloud water content, because the intensity of the radar return from a nuclear or natural cloud depends on the number and size of cloud particles, and also on the dielectric constants of the particle materials. The radar cross sections, and thus the radar return, of particles of a given size differ according as the particles consist of water, ice, or ice with a coating of water, i.e., wet ice. These differences, in turn, vary with both particle size and radar wave length.

Existing cloud models differ considerably in their purpose and in their physical and computational level of complexity. The SHELL model and computer program is a two-dimensional hydrodynamic model. The region of space in which the cloud develops is covered by a fixed (Eulerian) axisymmetric grid. To compute the cloud history, the mass, momentum, and energy conservation equations are solved for each zone or cell in the grid, in a sequence of discrete time steps covering the period of the cloud history. Versions of SHELL are available which compute the concentrations of dust and water in the cloud. In particular, the SHELL-WV program computes the concentrations of dry air, water vapor, liquid water, and ice. The condensed water is assigned to a single arbitrary particle size. The possible change in particle size and the evolution of a particle-size distribution are not considered.

Associated with SHELL is the DUSTY program which computes the trajectories of particles of specified mass in the flow field computed by SHELL. Again, the possible changes in particle size during the trajectories are not considered.

1.3 OBJECTIVE AND GENERAL APPROACH

The objectives of the present study were to review the physical processes affecting growth of water and ice particles in nuclear clouds, to identify significant growth mechanisms, and to develop a computer program modeling particle growth, suitable for eventual incorporation into the SHELL program.

The general approach was to make both the review of particle physics and program development open-ended. The AEROSOL program described in this report is intended to be combined with the SHELL program and the DUSTY program, to form a SUPER-SHELL program. SHELL computes cloud hydro- and thermodynamics. DUSTY computes particle trajectories. AEROSOL will be interactive with these programs, and will communicate with them through COMMON blocks. At each time step, for each space zone, AEROSOL will use data generated by the other programs, and return new data to them. For instance, AEROSOL will use the gas temperature and pressure computed by SHELL, and the particle velocities and falling rates computed by DUSTY. As a future development, additional particle growth mechanisms may be incorporated in AEROSOL, for instance, turbulence effects. The particle allocation (bookkeeping) procedures in AEROSOL are designed to accept any such mechanisms.

1.4 PLAN OF THIS REPORT

Particle growth processes are reviewed and processes to be programmed are given mathematical formulation in Section 2. The algorithms for representing particle growth by a specified number of discrete particle-size classes are also developed in this section.

The AEROSOL computer program is described in Section 3. This section also contains instructions for the intended incorporation of AEROSOL into SHELL.

Section 4 describes test computations made with AEROSOL. These computations were made to ensure that the program was operating correctly.

Section 5 gives recommendations and procedures for further development of the AEROSOL program, including extension to growth of multi-material particles, and consideration of additional growth mechanisms.

The Appendix contains a listing of the AEROSOL program. The Bibliography lists several references on cloud physics which give the background to the particle-growth equations used in AEROSOL.

SECTION 2

PHYSICAL PROCESSES AND MATHEMATICAL FORMULATION OF PARTICLE GROWTH

2.1 PHYSICAL PROCESSES

The size of water-substance particles can change by condensation/evaporation of water vapor, and by agglomeration (also called coagulation) and breaking of the particles. Both these types of mechanism change the particle-size distribution. The distribution within a fixed volume of space, such as a cell in an Eulerian computational grid, also changes as existing particles enter and leave the volume. Thus the size distributions are affected by condensation, coagulation, and transport processes. The three types of process are interactive, and in addition are affected by phase changes, e.g., freezing and solution processes, which do not directly change particle size.

Attention is centered on air bursts, for which entrained atmospheric moisture contributes most of the eventual particulate mass. For land surface bursts, the cloud particles consist mainly of so-called dust, i.e., soil and rock material, and for sea surface bursts, salt and the ocean water as well as atmospheric moisture, may play important parts in particle growth. In the present treatment, particles are taken as consisting principally or entirely of water.

In a review of water-particle growth processes, the question arises whether any such processes are important in nuclear clouds which are not important, and possibly non-existent, in natural clouds. Nuclear clouds, even after they have cooled to the water-condensation point, differ from natural clouds in their extreme turbulence, high updraft velocities, and rapid temperature changes. The intensities of these phenomena in high-yield nuclear clouds far exceed the intensities in even the largest natural convective clouds. Thus coagulation by turbulent acceleration may contribute significantly to particle growth in nuclear clouds, while in natural clouds this mechanism is generally much less important than coagulation due to gravitational acceleration, i.e., differential falling rates of large and small particles.

Would it be possible for droplets or crystals of diameter ten to a hundred microns to grow to precipitation size, i.e., diameter of order at least a thousand microns, by condensation alone, because of the intense updrafts and rapid cooling of the nuclear cloud? Such purely condensational growth does not occur in natural clouds. The answer is probably negative. The rapid cooling and resulting supersaturation of the air tend to activate additional condensation nuclei. There is not time for more condensing vapor to diffuse to the droplet surface. Thus growth is diffusion-limited. Also, the increased droplet or crystal population results in more frequent collisions; and thus more particle growth by agglomeration. However, the intense updrafts and turbulent mixing do prolong the residence times of particles in the nuclear cloud, and thus permit an increase in growth by condensation. This effect on growth is perhaps analogous to the growth of hailstones in updrafts in natural convective clouds.

2.2 CONDENSATION/EVAPORATION PROCESSES

In modeling water condensation, it is assumed that condensation nuclei already exist. Even in the natural atmosphere the concentration of nuclei is much greater than the concentration of droplets. Thus only a very small fraction of the nuclei are involved in droplet formation. This oversupply of nuclei will be at least equally true in the nuclear cloud even in the case of an air burst for which these nuclei will be provided primarily by the recondensed device materials. Surface bursts, of course, provide a much larger supply of nuclei.

For a single, spherical water or ice particle of radius r, the rate of change of particle mass, m, due to evaporation/condensation is given by

$$\frac{dm}{dt} = 4\pi r D(\rho_a - \rho_s)(VM)$$

where

D = diffusivity of water vapor in air

ρ_a = water vapor density in the ambient gas

ρ_s = water vapor density at particle surface

VM = ventilation factor for mass transfer

$VM = 1 + CVM\ Re^{1/2}\ Sc^{1/3}$

Re is the Reynolds number $2rv/\nu$, where v is relative particle velocity and ν is gas viscosity. Sc is the Schmidt number ν/D. CVM is a non-dimensional factor of order 0.3. The value of ρ_s varies with the temperature at the particle surface. Therefore, unless certain simplifying assumptions are made, as described below, it is necessary to solve the heat transfer and mass transfer equations simultaneously. The rate of change of particle heat content H due to evaporation/condensation is given by

$$\frac{dH}{dt} = 4\pi r K(T_s - T_a)(VH)$$

K = heat conductivity of air

T_a = temperature in the ambient gas

T_s = temperature at particle surface

VH = ventilation factor for heat transfer,

$VH = 1 + CVH\ Re^{1/2}\ Pr^{1/3}$

Pr is the Prandtl number $C_p \nu / K \rho_a$, where C_p is the specific heat of the gas. CVH is of order 0.3.

The complexity of solving the mass and heat transfer equations lies largely in the interaction of surface temperature and surface vapor density. If the particles are micron-size or smaller, vapor pressure at the surface is increased significantly by surface tension. Thus, for instance, in an atmosphere at 100% relative humidity larger drops may grow at the expense of smaller ones.

If droplets contain dissolved salts or other contaminants, then vapor pressure varies with the concentration and properties of these contaminants. Thus the phase transition from dry to wet particles can occur at less than 100% relative humidity due to lowering of vapor pressure over a solution. Vapor-pressure data is available for only a limited number of solutions of pure compounds, while nuclear air-burst and land-burst particles may contain a variable mixture of metal oxides and silicates and other ground materials.

It has been assumed in the development of the AEROSOL program that that particles consist of pure water or ice. Surface tension effects are neglected. Under these circumstances, the rates of mass transfer and heat transfer to a particle are directly related by

$$\frac{dH}{dt} = -L \frac{dm}{dt}$$

Here L is the latent heat of evaporation or sublimation, according as the drop is liquid or frozen. It is further assumed that water-vapor pressure at the drop surface is the saturation pressure of water vapor at the drop surface temperature. The quantities $\rho_a - \rho_s$ and $T_a - T_s$ can then be related to each other, and the mass growth rate can be defined entirely in terms of known ambient quantities. The mathematical procedure involves manipulation of the ideal gas law for the water vapor densities, and use of the Clausius-Clapeyron equation to eliminate the drop-surface parameters. For details see the references cited in the Bibliography.

The resulting particle-growth equation, after making certain approximations, can be written

$$\frac{dm}{dt} = \frac{4\pi r D(VM)\rho_e(S - 1)}{1 + DL^2 \rho_e M_w (VM)/RT_a^2 K(VH)}$$

In addition to the symbols previously defined, R is the ideal gas constant, M_w is the molecular weight of water, and S is the saturation ratio, or ratio of ambient vater-vapor pressure ρ_a to saturation water-vapor pressure ρ_e at the cloud gas temperature, T_a. Thus condensation and evaporation occur according as S exceeds or is less than unity, respectively.

Particle density is taken as that of liquid water. Since ice is about 9% less dense, an ice particle has about 3% greater radius than a water drop of the same mass. Thus use of constant water density tends to underestimate the rate of evaporation/condensation of ice particles by about 3%. Since the program uses the correct values of vapor pressure and latent heat for water and ice, the net error should be considerably less than 3%.

2.3 AGGLOMERATION PROCESSES

Very small, sub-micron processes collide and adhere primarily because of Brownian motion. The largest water and ice particles, of diameters in the millimeter range, collide with smaller particles primarily due to gravity, that is, because of differential falling rates of larger and smaller particles. In the size range between microns and millimeters several processes may operate to cause agglomeration. Electrical attraction may cause agglomeration between particles bearing different charges.

Such charge effects may be enhanced by ionizing radiation from the fission products and other radionuclides carried by particles in the nuclear cloud.

Two types of turbulence mechanism cause collision of particles: turbulent shear and turbulent acceleration. Because different nearby elements of a turbulent fluid move with different velocities, particles moving with the fluid may collide due to turbulent shear. Because particles of different sizes have different inertia, two such neighboring particles may collide due to turbulent acceleration of a fluid element. Thus turbulent acceleration acts like a randomly directed gravity to produce collisions between particles of different sizes.

Agglomeration may produce nuclei, for further condensation, consistint of a mixture of different materials. The surface of an agglomerated nucleus will contain cracks and cavities which are favored condensation sites. If the mixture includes soluble and insoluble materials, then above the phase transition for the soluble material, the particle behaves as a solution droplet. The presence of the insoluble components enhances the effectiveness of the soluble salts by increasing the particle size and therefore the mass rate of condensation. Thus agglomeration and condensation interact in particle growth.

Not all particles on a collision course actually collide, and not all colliding particles actually adhere to each other. In the first case, aerodynamic forces may deflect one particle around another. On the other hand, the deflecting forces may be balanced or outweighed by electrical attraction between two particles. As to adhesion efficiencies, some particle-growth model calculations assume that colliding ice particles do not adhere, while collisions between an ice particle and a water particle do result in adhesion.

Large drops, of diameter several millimeters, are likely to break up into two or more smaller drops. Small ice particles may split up due to stresses caused by freezing and temperature changes. The resulting multiplication of ice particles may contribute to condensational growth, because two small ice particles will accrete more water vapor by condensation than one large particle of the same total mass.

In the formulation of agglomeration in the AEROSOL program, particle breakup is neglected. Two agglomerating, spherical particles are treated as forming a single, larger spherical particle. Collision-efficiency and adhesion effects are represented by a collision-efficiency factor which in test computations was taken as unity. For developmental purposes the collision mechanisms incorporated in the program were Brownian movement and gravity. The mathematical formulation of agglomeration is described in Section 2.5, "Particle-Size Classification Algorithms."

2.4 TRANSPORT PROCESSES

Particles can move into and out of a fixed volume of space such as a cell of the SHELL Eulerian hydrodynamic computation, due to two types of mechanisms. The first mechanism is that particles tend to move with the fluid. This particle motion occurs in steady fluid flow, and, to the extent that particle inertia can be neglected, also in accelerated flow. Secondly, particles move relative to the fluid, if the particles, the fluid, or both are subject to acceleration. Since large particles fall faster than small ones, they will enter and leave the fixed volume at different rates. Also, non-gravitational acceleration will move large and small particles into and out of the volume at different rates.

2.5 PARTICLE-SIZE CLASSIFICATION ALGORITHMS

For computational purposes, the particle-size distribution is represented by a set of discrete size classes. The smallest particles are assigned to the first class containing particles of mass m(1). Particle mass doubles from one class to the next so that $m(i) = 2m(i-1)$. The number of particles in class i, per unit volume, is $n(i)$. There are N classes, and N is chosen as large as required. For instance, $N = 30$ spans a mass range of 2^{30}, or a particle-diameter range of about one thousand, as from ten microns to one centimeter.

2.5.1 Condensation/Evaporation. Particles grow or shrink by condensation or evaporation as described by the final equations for $\frac{dm}{dt}$ given in Section 2.2. Thus, in a time interval Δt the mass of particles of class i changes by an amount $\Delta m(i)$, where

$$\Delta m(i) = \frac{dm}{dt} \Delta t$$

and the values of m, radius r, etc., appropriate to class i are used. However, the mass per particle in class i retains its fixed value $m(i)$, so that the particle of mass $m(i) + \Delta m(i)$ must now be allocated partly to the next larger or smaller class, i.e., to class $i+1$ or class $i-1$. The following allocation method was developed. In a time step Δt, the number of particles $n(i)$ in class i changes by an amount

$$\Delta n(i) = \mp \frac{n(i)\Delta m(i)}{m(i+1) - m(i)} + \max\left(0, \frac{n(i-1)\Delta m(i-1)}{m(i) - m(i-1)}\right)$$
$$+ \max\left(0, -\frac{n(i+1)\Delta m(i+1)}{m(i+1) - m(i)}\right)$$

In the first term on the right side of the equation, the minus and plus signs are used according as $\Delta m(i)$ is positive or negative. Thus the term is always negative, since any change in size of an i class particle must result in some of its mass being allocated to the next smaller or larger class. If $\Delta m(i-1)$ is positive, $n(i)$ thereby increases, as shown in the second term. If $\Delta m(i+1)$ is negative, $n(i)$ increases as shown in the third term. If these two Δ-amounts have the opposite signs they do not affect n(i), but instead affect classes i-2 and i+2, respectively.

Class number one requires special treatment because there is no class i-1. To take care of this case, n(0) is defined as zero. Furthermore, particles are not allowed to shrink below mass m(1), which is treated as a dry condensation nucleus. Therefore, if Δm(1) is negative, only the third term above is non-zero:

$$\Delta m(1) = \max\left(0, \frac{n(2)\,\Delta m(2)}{m(2) - m(1)}\right)$$

In the foregoing algorithm, the total gain in particle mass in time Δt is exactly equal to the mass of water vapor condensing, summed over all size classes, and the total number of particles is unchanged.

2.5.2 Agglomeration. If two particles of class i agglomerate, evidently n(i) is reduced by 2 and some other class n(j) is increased. If an i and a j particle agglomerate, adjustments must be made in n(i) and n(j) and in the classes to which the new particle is assigned. The frequency of collision of i and j particles, per unit concentration of each class, is called F(i,j). Then the number of such collisions per unit time, per unit volume, is F(i,j)n(i)n(j). The following new algorithm was developed which conserves total particle mass and reduces particle number by one for each collision. In a time Δt, n(i) changes by agglomeration by an amount Δn(i):

$$\Delta n(i) = -\sum_{j=1}^{i-1} F(i,j)n(i)n(j)\,2^{j-i} - \sum_{j=i}^{N} F(i,j)n(i)n(j)$$
$$+ \sum_{j=1}^{i-1} F(i-1,j)2^{j-i}\,n(i-1)n(j)$$

Thus, a j,i collision, for $j \leq i$, reduces n(j) by 1, reduces n(i) by 2^{j-i}, and increases n(i+1) by 2^{j-i}.

2.5.3 Total Change in Particle-Size Distribution. The total change in size distribution in a time Δt, due to both condensation and agglomeration, is given by the sum of the $\Delta n(i)$ for the two mechanisms, as specified in Sections 2.5.1 and 2.5.2, respectively. In addition, the n(i) may change by transport processes as described in Section 2.4. It is intended that transport effects be computed by the DUSTY portion of the eventual SUPER-SHELL program mentioned in Section 1.3.

SECTION 3
DESCRIPTION OF THE AEROSOL PROGRAM

3.1 GENERAL APPROACH AND PROGRAM STRUCTURE

The AEROSOL program is intended primarily for incorporation into the SHELL/DUSTY system. The program can be run independently for development and checkout purposes, if initial values of variables, values of cloud parameters and physical constants are specified. All these variables are in COMMON so that they may be updated either within AEROSOL or through the appropriate subroutine of SHELL or DUSTY which contains the same COMMON statements.

The program is designed to permit incorporation of additional particle-growth mechanisms besides those now computed. Thus, it includes flags (true-false variables) which may be set to compute or omit ventilation factors, and surface-tension effects on evaporation/condensation. The logic for these computations may subsequently be developed and inserted when feasible. Similarly, the collision frequencies contributing to agglomeration are computed in a separate subroutine. The logic for collision frequencies due to Brownian motion, electrostatic attraction, turbulent acceleration, gravity, for collision efficiency and for particle breakup may be inserted step-by-step.

AEROSOL consists of the following elements. The main program, TEST, includes most of the variable data and "flag" options. TEST calls subroutines SETUP and AEROSOL. SETUP includes values of physical constants. AEROSOL contains the evaporation/condensation equations and the tests for most of the flags and options. AEROSOL calls subroutine NCONCN or alternatively, CONCEN, which reclassifies particles at each time step, and updates the size distribution to allow for the effects of condensation and agglomeration. CONCEN calls subroutine COLLIS to compute the collision frequencies used in the agglomeration equations. COLLIS calls function FGT to compute the collision frequencies due to different velocities or falling rates of particles of different size classes. Brief descriptions of these subroutines are given below.

3.2 TEST

TEST is the main program for AEROSOL. It serves primarily as an executive program. It is used to (1) define input data, (2) define values of flags that are set as options, (3) define certain auxiliary variables as functions of input data, (4) initialize the computation by calling SETUP, (5) call AEROSOL and update problem time and terminate the computation when the specified problem time or number of time steps is reached, (6) print values of some of the variables.

When AEROSOL is incorporated in SHELL, purposes (1) and (6) will be performed by SHELL. The auxiliary variables (3) can be computed by SETUP. Problem-time control (5) must be compatible with the cloud computation and therefore will be replaced by SHELL time control. If the data supplied by SETUP is available in the main program, (4) is unnecessary. The values of flags (2) can either be given as part of the SHELL data, or be incorporated semi-permanently as data statements in AEROSOL. Thus, it will be feasible for SHELL to call subroutine AEROSOL directly and TEST can be discarded.

3.3 SETUP

SETUP is called once by TEST at the start of computation. It contains the values of physical constants as data statements. These are placed in SETUP so that the rest of the operating program, subroutine AEROSOL, etc., can be used with any consistent system of units. The data now given in SETUP are in cgs units. For SHELL operation all these data should be available from the main program through COMMON. SETUP also contains the definition of the class-to-class difference in particle mass, DIFCM(I-1) = CM(I) - CM(I-1). For SHELL operation the definition of particle class radius RAD(I) should be transferred to SETUP from TEST.

3.4 AEROSOL

AEROSOL is the principal operating subroutine. It is called at each time step by TEST. For SHELL operation, AEROSOL will be called directly by the appropriate subroutine of SHELL.

AEROSOL computes, for each size class, the rate of mass change due to evaporation/condensation. It also computes the corresponding rate of heat transfer. Before making these computations, it checks the status of the flags IMPURE and PSMALL. A TRUE value for IMPURE indicates that solute effects are to be allowed for. A TRUE value for PSMALL indicates that small particle effects, i.e., curvature and surface tension are to be allowed for. The TRUE logic has not yet been developed; hence a TRUE answer stops the program. If both these flags are set to FALSE, then heat transfer is taken as proportional to mass transfer (Section 2.2). AEROSOL also tests whether particles are liquid or frozen and resets the corresponding flags, FROZEN and TFFLAG.

AEROSOL calls the particle-classification subroutine NCONCN, or alternatively, CONCEN, which adjusts the size distribution for changes due to both evaporation/condensation and agglomeration.

3.5 NCONCN

Subroutine NCONCN is called by AEROSOL. NCONCN calls COLLIS to determine the collision frequencies, CF(I,J), between each pair of particle size classes. The term collision frequency here is taken to allow for collision efficiency, sticking coefficients, etc., so that CF(I,J) are the effective collision efficiencies. NCONCN reallocates mass between size classes to take into account evaporation/condensation of particles of each class as computed in AEROSOL, and destruction and creation of particles by agglomeration, at the frequencies computed in COLLIS. The allocation scheme ensures that the number of particles is conserved in evaporation/condensation and that the mass of particles is conserved in agglomeration and that each collision reduces particle number by exactly one unit.

CONCEN is a similar, alternative subroutine. It uses an earlier allocation scheme which lacks the exact treatment of particle number in agglomeration. Furthermore, it may be valid only for condensing, not evaporating particles, until revisions are made to bring it into line with NCONCN. Use of NCONCN is therefore recommended.

3.6 COLLIS

Subroutine COLLIS is called by NCONCN or CONCEN. It computes the collision frequencies CF(I,J) of all pairs of classes I,J. At present, the collision frequencies specified in COLLIS are those due to Brownian motion, FB, and due to gravity, FGT. COLLIS calls function FGT(I,J) to compute gravitational collision frequencies. Collision frequencies due to other mechanisms, such as turbulence effects and zone-to-zone variations in velocities and accelerations, as computed by SHELL, can be inserted in the CF(I,J) computation. If collision efficiencies and particle breakup frequencies are considered, they can also be inserted in COLLIS.

3.7 FGT

Function FGT(I,J) is called by COLLIS to compute collision frequencies between particles of classes I and J, due to differences in either gravitational fall rates VG(I) or velocities V(I) between I and J particles. VG and V are in COMMON and it is intended that their values will be initialized and updated by sub-program DUSTY. For stand-alone use of AEROSOL, equations to compute falling rates should be inserted. At present, FGT contains the dummy value FGT = 0.

SECTION 4
TEST COMPUTATIONS

4.1 TYPES OF TEST MADE

Test computations were performed to verify that the programming correctly reproduced the algebraic form of the particle-growth equations, and that certain of the internal program controls operated correctly. The controls tested included those that specify whether particles were frozen or liquid, and those that determine the time step DELTIM used in integrating the particle-growth equations.

For most of the tests, the numerical values used for input data were as shown in the listing of TEST, except that for ambient air temperature, TAMB, the two values 273.5 and 273. were both used to test the freeze/melt logic, since the freezing point used was TF = 273.16 as shown in the listing of SETUP. Other physical constants were also as shown in SETUP.

Hand computations were made at the first time step, of the rate of condensation of class 1 particles, and of the Brownian collision frequency. The printouts were checked against the hand computation.

4.2 FLAGS TESTED

Test runs were made with both TRUE and FALSE values of NAGLOM, TFIX, CWF, FROZEN, and SKIP. NAGLOM omits the agglomeration computation, i.e., the collision frequencies are set to zero. If SKIP = FALSE the condensation/evaporation computation is in effect omitted (skipped). SKIP is not an input option, but can be set to FALSE by proper choice of the input CWF and of SPEMIN, the threshold value of saturation ratio S.

When TFIX is FALSE, the value of time step DELTIM is halved or doubled from its initial value until the fractional change in mass, of the smallest particle, of mass CM(1), in a time DELTIM, is between C/2 and C. The value C = .1 was used, i.e., DELTIM was set to permit between 5% and 10% mass-change in the smallest particles. With the input data shown in the listing, DELTIM is halved six times from its initial value of 0.1 seconds, before the test is passed. The data includes a supersaturation value of 10% which was chosen for test purposes and is not to be considered physically realistic.

If CWF = FALSE, the program assumes that no condensed water is present. This option is intended for use when only particles of the smallest size, i.e., class 1, are present. The convention is that class 1 particles are dry nuclei which cannot evaporate. If they were permitted to shrink by evaporation, smaller-size classes would be needed in the allocation scheme. If they were permitted to disappear completely by evaporation, an additional algorithm would be needed to assign condensing vapor if water started to condense at a later time step. CWF is automatically reset to TRUE after any time step in which the mass of a particle of at least one class increases. CWF is automatically reset to FALSE after a time step such that all size classes except class 1 are empty of particles and also saturation ratio S was less than the specified threshold value.

FROZEN was given initial TRUE and FALSE values with TAMB set to values 273.5 and 273, i.e., just above and below the freezing point TF = 273.16, thus giving FALSE and TRUE values of TFFLAG. If, for instance, FROZEN = FALSE and TFFLAG is found to be TRUE, then the vapor-pressure constants and latent heat value are reset from liquid-water to ice values, and the release of heat of fusion is computed. The other logical combinations are treated similarly.

4.3 MASS AND NUMBER CONSERVATION

It was verified that total particle mass remains constant in agglomeration, that total particle number remains constant in evaporation condensation (because each particle is assumed to contain a non-volatile condensation nucleus which remains after all water has evaporated), and that each collision (at 100% efficiency) reduces the total number of particles by one. Total mass of particles is defined as SUMA in TEST and is printed by TEST. Total number of particles is the sum of all CN(I). For checkout purposes, this sum was computed and printed by TEST.

4.4 COMPUTATIONAL DIFFUSION OF THE SIZE DISTRIBUTION

The particle-size classes are Eulerian, that is, each size class represents particles of a fixed size. If the size distribution initially consists of class 1 particles only, then if any condensation takes place in the first time step, the effect of condensation is represented by the creation of a few class 2 particles. An alternative Lagrangian classification scheme would be to increase slightly the size represented by class 1, after the first time step. The terms Eulerian and Lagrangian are used in analogy to fixed-grid and fixed-mass cells in hydrodynamic computations. In the present, Eulerian method, if at time step 2 class 2 particles grow by condensation, then some class 3 particles are created. After 10 time steps there will be particles of classes 1 through 10, even though a single particle of class 1 size might not even have grown to class 2 size. Thus, the particle size distribution tends to diffuse through the size classes. The effect appears in computing agglomeration as well as condensation. This effect is similar to mass diffusion in Eulerian hydrodynamics.

As an example of the diffusion effect, with the test data shown in the listing, a class 1 particle has mass CM(1) = 5.236 E-13 while CM(2) = 1.047 E-12. The mass condensation rate for class 1 is 2.930 E-11, so that it would take about 1.8 E-2 seconds for the class 1 particle to reach class 2 size. This time interval is nearly 12 of the time steps DELTIM used in the computation, with DELTIM controlled to permit a 10% mass growth per time step.

The rate of advance of the diffusion front is just one class per time step, no matter how small the time step. However, the possible actual error produced in the size distribution by the Eulerian method is very small. In the present system of sizes, class I +1 has twice the mass per particle that class I does. The resulting diffusive front is very steep. After 10 time steps the concentration, CN, at the front may decrease by a factor of over 1000 per size class. For instance, in one run for condensation alone without agglomeration, the values were of order CN(2) = 1.E2, CN(3) = 4.E0, CN(4) = 6.E-2, down to CN(9) = 8.E-17, CN(10) = 6.E-21, CN(11) = 1.E-25, CN(12) = 0.

The point is that the Eulerian method gives both the correct mean mass of a particle, and the correct number of particles, and that the smearing of the distribution amounts to a negligible fraction of the total mass.

Furthermore, the alternative Lagrangian method is not feasible if agglomeration is to be computed, because it results in an increase in the number of size classes at each time step. Thus, an Eulerian allocation scheme is a practical necessity for computing development of a particle size distribution.

SECTION 5

RECOMMENDATIONS FOR FURTHER DEVELOPMENT

AEROSOL should be extended to handle the simultaneous presence of liquid-water and ice particles in the same computational cell. The appropriate treatment may be to carry two different species of particles, or, in each cell, to allocate all water particles to either the liquid or the frozen state, with the temperature adjusted for latent-heat changes so as to conserve total energy.

Particles from land-surface bursts consist initially mainly of soil or rock materials, on which moisture gradually condenses. AEROSOL should be extended to such multi-material particles. Interactions between dust and water should be considered. If the dust fraction of total particle mass is significant, an averaging method must be developed so that all particles of one size class have the same density. A statistical algorithm may be required, to decide what fraction of the dry dust nuclei are activated at each time step in the condensation of water vapor.

Turbulence effects on agglomeration should be incorporated in the program. To generate turbulence variables for each computational cell, AEROSOL will have to look at the fluid velocities in the adjoining cells of the SHELL grid. Alternatively, the turbulence estimation routine may be incorporated directly in SHELL, and the turbulence parameters made available through COMMON. Collision-efficiency factors and drop-breakup frequencies should be included in the program on a simplified basis.

In addition to extensions of AEROSOL, test runs using a range of realistic burst and atmospheric conditions should be performed to detect possible program errors and to verify the realism and reliability of the SUPER-SHELL program.

BIBLIOGRAPHY

The following standard works on cloud physics were used as references on particle growth.

1. Fletcher, N. H., The Physics of Rainclouds, Cambridge University Press, 1962.

2. Mason, B. J., The Physics of Clouds, Oxford University Press, 1957.

The form given for condensational particle growth is based on that used in the following reference.

3. Bird, R. G., Stewart, W. E., and Lightfoot, E. N., Transport Phenomena, Wiley, 1960.

The following reports and articles were also used in formulating the particle-growth equations.

4. Danielsen, E. F., et al.,"Hail Growth by Stochastic Collection in a Cumulus Model," J. Atmos. Sci., Vol. 29, p. 135, January 1972.

5. Huebsch, I. O., "Relative Motion and Coagulation of Particles in a Turbulent Gas," USNRDL-TR-67-49, May 1967.

6. Koenig, L. R., "Numerical Modeling of Ice Deposition," RAND Corporation RM-5715-NSF, August 1968.

7. Ogura, Y., and Takahashi, T., "Numerical Simulation of the Life of a Thunderstorm Cell," Monthly Weather Review, Vol. 99, No. 12, p. 895, December 1971.

8. Slinn, W. G. N., and Gibbs, A. G., "The Stochastic Growth of a Rain Droplet," J. Atmos. Sci., Vol. 28, p. 973, September 1971.

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APPENDIX

LISTING OF THE AEROSOL PROGRAM

```
      PROGRAM TEST(INPUT,OUTPUT,TAPE8=INPUT,TAPE1=OUTPUT)               TES00000
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,  TES00100
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM                            TES00200
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,       TES00300
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP                                   TES00400
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,         TES00500
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,                  TES00600
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO                   TES00700
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,                    TES00800
     1RHOES,P                                                           TES00900
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),          TES01000
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),                       TES01100
     2CF(50,50),DMDT(50),STATE(50),VG(50)                               TES01200
C***********************************************************************TES01300
C                                                                       TES01400
C  VARIABLES NORMALLY SET BY 'SHELL'                                    TES01500
C                                                                       TES01600
C***********************************************************************TES01700
C                                                                       TES01800
C  FLAGS SET AS OPTIONS --                                              TES01900
C                                                                       TES02000
C***********************************************************************TES02100
C                                                                       TES02200
C-----------------------------------------------------------------------TES02300
C  CHANGE IN DROP HEAT CONTENT CONSIDERED                               TES02400
      DATA  CDHC   / .FALSE.        /                                   TES02500
C-----------------------------------------------------------------------TES02600
C  NO AGGLOMERATION CONSIDERED                                          TES02700
      DATA  NAGLOM / .FALSE.        /                                   TES02800
C-----------------------------------------------------------------------TES02900
C  PARTICLES CONTAIN IMPURITIES                                         TES03000
      DATA  IMPURE / .FALSE.        /                                   TES03100
C-----------------------------------------------------------------------TES03200
C  CONDENSATION/EVAPORATION IS INSTANTANEOUS                            TES03300
      DATA  INSTCN / .FALSE.        /                                   TES03400
C-----------------------------------------------------------------------TES03500
C  FREEZING/MELTING IS INSTANTANEOUS                                    TES03600
      DATA  INSTFM /  .TRUE.        /                                   TES03700
C-----------------------------------------------------------------------TES03800
C  CALCULATION IS INTERACTIVE WITH ATMOSPHERE                           TES03900
      DATA  INTRCT / .FALSE.        /                                   TES04000
C-----------------------------------------------------------------------TES04100
C  PARTICLE IS SMALL ENOUGH FOR SURFACE TENSION OR CURVATURE TO AFFECT  TES04200
C   WATER VAPOR DENSITY OVER SURFACE                                    TES04300
      DATA  PSMALL / .FALSE.        /                                   TES04400
C-----------------------------------------------------------------------TES04500
C  TIME STEP IS FIXED                                                   TES04600
      DATA  TFIX   / .FALSE.        /                                   TES04700
C-----------------------------------------------------------------------TES04800
C  VENTILATION FACTORS ARE SIGNIFICANT                                  TES04900
      DATA  VFSIG  / .FALSE.        /                                   TES05000
C-----------------------------------------------------------------------TES05100
C                                                                       TES05200
C***********************************************************************TES05300
C                                                                       TES05400
C  FLAGS THAT MAY BE RESET BY PROGRAM                                   TES05500
```

```
C                                                                       TES05600
C***********************************************************************TES05700
C                                                                       TES05800
C-----------------------------------------------------------------------TES05900
C  CONDENSED WATER PRESENT                                              TES06000
      DATA  CWF    / .TRUE.        /                                    TES06100
C-----------------------------------------------------------------------TES06200
C  PARTICLES ARE FROZEN                                                 TES06300
      DATA  FROZEN / .TRUE.        /                                    TES06400
C-----------------------------------------------------------------------TES06500
C                                                                       TES06600
C***********************************************************************TES06700
C                                                                       TES06800
C  VARIABLES THAT MAY BE SET, INITIALIZED OR UPDATED BY SHELL           TES06900
C   BUT MUST BE DEFINED HERE FOR STAND ALONE RUN                        TES07000
C                                                                       TES07100
C***********************************************************************TES07200
C                                                                       TES07300
C-----------------------------------------------------------------------TES07400
C  MAXIMUM PERMISSIBLE CHANGE PER TIME STEP                             TES07500
      DATA  C      / .1            /                                    TES07600
C-----------------------------------------------------------------------TES07700
C  PARTICLE CONCENTRATIONS                                              TES07800
      DATA  CN     / 1.0E6,49*0.0  /                                    TES07900
C-----------------------------------------------------------------------TES08000
C  KINEMATIC VISCOSITY OF AIR AT CONSTANT PRESSURE                      TES08100
C   CNU VALUE MATCHES P AND TAMB                                        TES08200
      DATA  CNU    / .14           /                                    TES08300
C-----------------------------------------------------------------------TES08400
C  TIME STEP VALUE                                                      TES08500
      DATA  DELTIM / .1            /                                    TES08600
C           SECONDS                                                     TES08700
C-----------------------------------------------------------------------TES08800
C  NUMBER OF TIME STEPS                                                 TES08900
      DATA  NSTEP  / 20            /                                    TES09000
C-----------------------------------------------------------------------TES09100
C  NUMBER OF PARTICLE CLASSES                                           TES09200
      DATA  NUMPAR / 20            /                                    TES09300
C-----------------------------------------------------------------------TES09400
C  PRESSURE                                                             TES09500
      DATA   P     / 1.013E6       /                                    TES09600
C           DYNES / CENTIMETER   2                                      TES09700
C-----------------------------------------------------------------------TES09800
C  RATIO BETWEEN MASS OF PARTICLES IN CONTIGUOUS CLASSES                TES09900
C   AGGLOMERATION LOGIC VALID ONLY FOR RATIO = 2.                       TES10000
      DATA  RATIO  / 2.            /                                    TES10100
C-----------------------------------------------------------------------TES10200
C  PARTICLE DENSITY                                                     TES10300
      DATA  RHOP   / 1.0           /                                    TES10400
C           GRAMS / CENTIMETER   3                                      TES10500
C-----------------------------------------------------------------------TES10600
C  WATER VAPOR DENSITY                                                  TES10700
C   10 PERCENT SUPERSATURATION AT TAMB = 273.                           TES10800
      DATA  RHOVA  / 5.34E-6       /                                    TES10900
C           GRAMS / CENTIMETER   3                                      TES11000
C-----------------------------------------------------------------------TES11100
```

```
C  WATER VAPOR DENSITY OVER DROP SURFACE                                TES11200
      DATA  RHOVS  / 50*0.0      /                                      TES11300
C         GRAMS / CENTIMETER   3                                        TES11400
C-----------------------------------------------------------------------TES11500
C  MINIMUM VALUE FOR TEST OF SATURATION RATIO                           TES11600
      DATA  SPEMIN / 1.0         /                                      TES11700
C-----------------------------------------------------------------------TES11800
C  AMBIENT AIR TEMPERATURE                                              TES11900
      DATA  TAMB   / 273.5       /                                      TES12000
C         DEGREES KELVIN                                                TES12100
C-----------------------------------------------------------------------TES12200
C  INITIAL TIME                                                         TES12300
      DATA  TIM    / 0.0         /                                      TES12400
C         SECONDS                                                       TES12500
C-----------------------------------------------------------------------TES12600
C  MAXIMUM TIME CONSIDERED                                              TES12700
      DATA  TIMMAX / 1.0         /                                      TES12800
C         SECONDS                                                       TES12900
C-----------------------------------------------------------------------TES13000
C  PARTICLE VELOCITIES                                                  TES13100
      DATA  V      / 50*0.0      /                                      TES13200
C         CENTIMETERS / SECOND                                          TES13300
C-----------------------------------------------------------------------TES13400
C                                                                       TES13500
      ONETRD=1./3.                                                      TES13600
      PI=4.0*ATAN(1.0)                                                  TES13700
C=======================================================================TES13800
C  DATA -- SMALLEST PARTICLE CLASS                                      TES13900
C  VALUE MEANS RAD(1) = .5E-4                                           TES14000
C=======================================================================TES14100
      CM(1)=4.*PI*(.125E-12)/3.                                         TES14200
      PRAD=.75/(PI*RHOP)                                                TES14300
      RAD(1)=(CM(1)*PRAD)**ONETRD                                       TES14400
      SUMA=CN(1)*CM(1)                                                  TES14500
      WRITE(1,1000)                                                     TES14600
 1000 FORMAT(1H1)                                                       TES14700
      WRITE(1,1100) SUMA                                                TES14800
 1100 FORMAT(/,20X,26HTOTAL MASS OF PARTICLES = ,E11.4,//)              TES14900
      I=1                                                               TES15000
      WRITE(1,1200) I,CM(I),I,RAD(I)                                    TES15100
 1200 FORMAT(20X,3HCM(,I2,4H) = ,E10.4,20X,4HRAD(,I2,4H) = ,E10.4,/)    TES15200
      DO 50 I=2,NUMPAR                                                  TES15300
      CM(I)=CM(I-1)*RATIO                                               TES15400
      RAD(I)=(CM(I)*PRAD)**ONETRD                                       TES15500
      WRITE(1,1200) I,CM(I),I,RAD(I)                                    TES15600
   50 CONTINUE                                                          TES15700
      CALL SETUP                                                        TES15800
      WRITE(1,1000)                                                     TES15900
      DO 10 I=1,NSTEP                                                   TES16000
      IF(TIM.GT.TIMMAX) STOP                                            TES16100
      SUMA=0.0                                                          TES16200
      SUMH=0.0                                                          TES16300
      CALL AEROSOL                                                      TES16400
      TIM=TIM+DELTIM                                                    TES16500
      WRITE(1,1300) I,TIM,DELTIM                                        TES16700
 1300 FORMAT(///,20X,12HITERATION = ,I3,5X,7HTIME = ,E10.4,5X           TES16800
```

```
     112HTIME STEP = ,E10.4)
      WRITE(1,1400)
 1400 FORMAT(///,20X,5HCLASS,5X,13HCONCENTRATION,5X,
     114HCHANGE IN MASS,10X,5HDM/DT,/,20X,
     25H-----,5X,13(1H-),5X,14(1H-),10X,5H-----)
      DO 5 J=1,NUMPAR
      WRITE(1,1500) J,CN(J),DELCM(J),DMDT(J)
 1500 FORMAT(20X,I3,8X,E12.4,6X,E12.4,7X,E12.4)
      IF(CN(J).LT.0.0) CN(J)=0.0
C=======================================================================
C  TOTAL PARTICLE MASS CONCENTRATION
C=======================================================================
      SUMA=SUMA+CN(J)*CM(J)
C
C=======================================================================
C  HEAT RELEASED IN TIME STEP
C=======================================================================
      SUMH=SUMH+DELHA(J)
C
    5 CONTINUE
      WRITE(1,1100) SUMA
      WRITE(1,1600) SUMH
 1600 FORMAT(/,20X,49HTOTAL HEAT RELEASED TO ATMOSPHERE IN TIME STEP = ,
     1 E11.4)
      WRITE(1,1700)
 1700 FORMAT(/,5X,110(1H*))
   10 CONTINUE
      STOP
      END
```

```
      SUBROUTINE AEROSOL
C
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,
     1RHOES,P
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),
     2CF(50,50),DMDT(50),STATE(50),VG(50)
C***********************************************************************
C
C  DEFINITION OF VARIABLES USED --
C
C    I.  FLAGS (TRUE OR FALSE VALUES ONLY) -- INDICATE THE FOLLOWING
C       CDHC ---- CHANGE IN DROP HEAT CONTENT CONSIDERED
C       CWF ----- CONDENSED WATER PRESENT
C       FIRST --- USED ON CLASS ONE ONLY
C       FROZEN -- A FROZEN PARTICLE (FREEZING CONSIDERED)
C       IMPURE -- PRESENCE OF IMPURITIES IN PARTICLE
C       INTRCT -- CALCULATION INTERACTIVE WITH ATMOSPHERE
C       INSTCN -- INSTANT CONDENSATION IS ASSUMED
C       INSTFM -- INSTANT FREEZING/MELTING IS ASSUMED
C       NAGLOM -- OMIT AGGLOMERATION
C       NCDHC --- NEGATIVE OF CDHC
C       NINTRC -- NEGATIVE OF INTRCT
C       NSPMFG -- NEGATIVE OF SPEMFG
C       NUM1 ---- NUMPAR = 1
C       NUM2 ---- NUMPAR = 2
C       PSMALL -- PARTICLE SMALL ENOUGH FOR SURFACE TENSION OR CURVATURE
C                 TO AFFECT WATER VAPOR DENSITY OVER SURFACE
C       SKIP ---- DO NOT SKIP CONDENSATION/EVAPORATION LOGIC
C       SPEMFG -- SATURATION RATIO EXCEEDS SPEMIN
C       TFIX ---- FIXED TIME STEP
C       TIMF ---- CHANGE IN TIME IS AN INPUT
C       VFSIG --- SIGNIFICANCE OF VENTILATION FACTORS
C
C   II.  REAL VALUED VARIABLES
C       C ------- MAXIMUM PERMISSABLE CHANGE PER TIME STEP
C       CK ------ CONDUCTIVITY OF HEAT IN AIR
C       CLF ----- LATENT HEAT OF FREEZING
C       CLL ----- LATENT HEAT OF VAPORIZATION OF WATER AT TEMPERATURE
C                 ZERO DEGREES CENTIGRADE
C       CLM ----- LATENT HEAT OF MELTING (ICE-LIQUID TRANSITION)
C       CM ------ MASS OF PARTICLE OF CLASS(I)
C       CMW ----- MOLECULAR WEIGHT OF WATER
C       CN ------ PARTICLE CONCENTRATION
C       CNU ----- KINEMATIC VISCOSITY OF AIR AT RHOVA AND TAMB
C       CP ------ SPECIFIC HEAT OF AIR AT CONSTANT PRESSURE
C       CSI ----- SPECIFIC HEAT OF ICE
C       CSW ----- SPECIFIC HEAT OF WATER
C       CVH ----- HEAT VENTILATION FACTOR COEFFICIENT
```

```
C       CVM ----- MASS VENTILATION FACTOR COEFFICIENT                   AER05600
C       D ------- DIFFUSIVITY OF WATER VAPOR IN AIR                     AER05700
C       DN ------ TOTAL D(CN)/DT                                        AER05800
C       DNDTAG -- D(CN)/DT FOR AGGLOMERATION                            AER05900
C       DNDTEC -- D(CN)/DT FOR EVAPORATION/CONDENSATION                 AER06000
C       DELCM --- CHANGE IN MASS OF PARTICLE                            AER06100
C       DELH ---- HEAT RELEASED BY CONDENSATION                         AER06200
C       DELHA --- HEAT RELEASED TO ATMOSPHERE                           AER06300
C       DELHD --- CHANGE IN DROP HEAT CONTENT                           AER06400
C       DELTIM -- TIME STEP                                             AER06500
C       DELTIS -- STANDARD INITIAL VALUE FOR DELTIM                     AER06600
C       DELWV --- CHANGE IN WATER VAPOR MASS                            AER06700
C       DMDT ---- DM/DT                                                 AER06800
C       ES ------ SATURATION VAPOR PRESSURE OF WATER AT TEMPERATURE TAMB AER06900
C       HD ------ HEAT CONTENT OF DROP                                  AER07000
C       NUMPAR -- NUMBER OF PARTICLE CLASSES                            AER07100
C       P ------- AMBIENT AIR PRESSURE                                  AER07200
C       PI ------ 3.14159 . . .                                         AER07300
C       PR ------ PRANDTL NUMBER OF THE GAS (AIR)                       AER07400
C       RAD ----- PARTICLE RADIUS                                       AER07500
C       RE ------ REYNOLDS NUMBER OF PARTICLE                           AER07600
C       RG ------ GAS CONSTANT                                          AER07700
C       RHOLS --- SATURATION WATER VAPOR DENSITY AT TEMPERATURE TAMB    AER07800
C       RHOP ---- PARTICLE DENSITY                                      AER07900
C       RHOVA --- WATER VAPOR DENSITY                                   AER08000
C       RHOVS --- WATER VAPOR DENSITY OVER DROP SURFACE                 AER08100
C       RHOW ---- DENSITY OF WATER                                      AER08200
C       S ------- SATURATION RATIO                                      AER08300
C       SC ------ SCHMIDT NUMBER OF THE GAS (AIR)                       AER08400
C       SPEMIN -- SPECIFIED MINIMUM VALUE OF S                          AER08500
C       TAMB ---- AMBIENT AIR TEMPERATURE                               AER08600
C       TIM ----- TIME                                                  AER08700
C       TSUR ---- DROP SURFACE TEMPERATURE                              AER08800
C       V ------- VELOCITY OF PARTICLE RELATIVE TO AIR                  AER08900
C       VISC ---- DYNAMIC VISCOSITY OF AIR                              AER09000
C       VH ------ VENTILATION FACTOR FOR HEAT TRANSFER                  AER09100
C       VM ------ VENTILATION FACTOR FOR MASS TRANSFER                  AER09200
C                                                                       AER09300
C***********************************************************************AER09400
      LOGICAL NINTRC,NCDHC,TIMF,SPFMFG                                  AER09500
      TFFLAG=TAMB.LT.TF                                                 AER09600
      IF(FROZEN.OR.TFFLAG) GO TO 300                                    AER09700
C=======================================================================AER09800
C  SET CONSTANTS TO LIQUID VALUES                                       AER09900
C=======================================================================AER10000
      WRITE(1,1000)                                                     AER10100
 1000 FORMAT(////,25X,10(1H*),8H LIQUID ,10(1H*))                       AER10200
    1 A=AL                                                              AER10300
      B=BL                                                              AER10400
      CLN=CLL                                                           AER10500
      CSU=CSW                                                           AER10600
C                                                                       AER10700
C=======================================================================AER10800
C  TETENS EQUATIONS FOR SATURATION VAPOR PRESSURE IN CGS                AER10900
C=======================================================================AER11000
    2 ES=ESI*EXP(A*(TAMB-273.16)/(TAMB-B))                              AER11100
```

```
C                                                                       AER11200
      WRITE(1,1100) ES                                                  AER11300
 1100 FORMAT(/,25X,37HSATURATION VAPOR PRESSURE OF WATER = ,E10.4)      AER11400
C                                                                       AER11500
      RHOES=ES*CMW/(RG*TAMB)                                            AER11600
      RHOESF=RHOES*.99                                                  AER11700
      S=RHOVA/RHOES                                                     AER11800
      WRITE(1,1200) S                                                   AER11900
 1200 FORMAT(/,25X,19HSATURATION RATIO = ,E10.4)                        AER12000
      SPEMFG=S.GE.SPEMIN                                                AER12100
      SKIP=SPEMFG.OR.CWF                                                AER12200
C=======================================================================AER12300
C  IF NO CONDENSED WATER AND S BELOW CONDENSATION THRESHOLD             AER12400
C   THEN BYPASS EVAPORATION/CONDENSATION COMPUTATION                    AER12500
C=======================================================================AER12600
      IF(.NOT.SKIP) GO TO 950                                           AER12700
      FIRST=.TRUE.                                                      AER12800
C=======================================================================AER12900
C  'INSTCN' LOGIC NOT YET DEFINED                                       AER13000
C=======================================================================AER13100
      IF(INSTCN) GO TO 200                                              AER13200
C=======================================================================AER13300
C  '.NOT.INSTEM' LOGIC NOT YET DEFINED                                  AER13400
C=======================================================================AER13500
      IF(.NOT.INSTEM) GO TO 700                                         AER13600
      NCDHC=.NOT.CDHC                                                   AER13700
    3 DRHOVA=0.0                                                        AER13800
      DO 900 I=1,NUMPAR                                                 AER13900
      DRHO=RHOVA-RHOVS(I)                                               AER14000
C=======================================================================AER14100
C  'IMPURE' AND 'PSMALL' LOGIC NOT YET DEFINED                          AER14200
C=======================================================================AER14300
      IF(IMPURE) GO TO 400                                              AER14400
      IF(PSMALL) GO TO 500                                              AER14500
      IF(VFSIG) GO TO 70                                                AER14600
      VM=1.                                                             AER14700
      VH=1.                                                             AER14800
C=======================================================================AER14900
C  DRHO = RHOVA - RHOVS                                                 AER15000
C=======================================================================AER15100
    5 DRHO=RHOES*(S-1.)/(1.+(D*CLN*CLN*RHOES*CMW*VM/                    AER15200
     1(RG*TAMB*TAMB*CK*VH)))                                            AER15300
      FORPIR=4.*PI*RAD(I)                                               AER15400
C=======================================================================AER15500
C  GROWTH RATE OF PARTICLE                                              AER15600
C=======================================================================AER15700
      DMDTI=FORPIR*D*DRHO*VM                                            AER15800
C                                                                       AER15900
C=======================================================================AER16000
C  HEAT RELEASE RATE OF PARTICLE                                        AER16100
C=======================================================================AER16200
      DHDT=DMDTI*CLN                                                    AER16300
C                                                                       AER16400
      TSUR(I)=DHDT*(1./(FORPIR*CK))*(1./(1.+VH))+TAMB                   AER16500
   10 DELCMI=DMDTI*DELTIM                                               AER16600
      IF(TFIX) GO TO 15                                                 AER16700
```

```
      IF(FIRST) GO TO 50                                                AER16800
   15 CMI=CM(I)+DELCMI                                                  AER16900
C=======================================================================AER17000
C  TO TREAT CLASS 1 PARTICLES AS DRY NUCLEI, SET                        AER17100
C   NEGATIVE DELCMI TO ZERO FOR I = 1                                   AER17200
C=======================================================================AER17300
      CNI=CN(I)                                                         AER17400
   20 DELH=CLN*DELCMI                                                   AER17500
      DELHDI=0                                                          AER17600
      IF(NCLHC) GO TO 30                                                AER17700
C=======================================================================AER17800
C  IF FROZEN USE ICE VALUE FOR CSW                                      AER17900
C=======================================================================AER18000
      DELHDI=CSO*DELCMI*TSUR(I)                                         AER18100
C                                                                       AER18200
C=======================================================================AER18300
C  TOTAL HEAT RELEASED BY CLASS                                         AER18400
C=======================================================================AER18500
   30 DELHA(I)=(DELH-DELHDI)*CNI                                        AER18600
      DRHOVA=DRHOVA-CNI*DELCMI                                          AER18700
      GO TO 80                                                          AER18800
C=======================================================================AER18900
C  TEST TIME STEP                                                       AER19000
C=======================================================================AER19100
   50 DLCMCM=DELCMI/CM(I)                                               AER19200
      IF(ABS(DLCMCM).LE.C) GO TO 52                                     AER19300
      DELTIM=DELTIM/2.                                                  AER19400
      GO TO 10                                                          AER19500
   52 IF(ABS(DLCMCM).LE.C/2.0) GO TO 60                                 AER19600
C=======================================================================AER19700
C  TIME STEP ALL RIGHT                                                  AER19800
C=======================================================================AER19900
      FIRST=.FALSE.                                                     AER20000
      GO TO 15                                                          AER20100
   60 DELTIM=DELTIM*2.                                                  AER20200
      GO TO 10                                                          AER20300
C=======================================================================AER20400
C  COMPUTE VENTILATION FACTORS                                          AER20500
C=======================================================================AER20600
   70 SQRTRE=SQRT(2.*RAD(I)*V(I)/CNU)                                   AER20700
      SC=CNU/D                                                          AER20800
      PR=CP*CNU/(CK*RHOVA)                                              AER20900
      VM=1.+CVM*SQRTRE*SC**ONETRD                                       AER21000
      VH=1.+CVH*SQRTRE*PR**ONETRD                                       AER21100
      GO TO 5                                                           AER21200
C                                                                       AER21300
   80 CONTINUE                                                          AER21400
      DELCM(I)=DELCMI                                                   AER21500
      DMDT(I)=DMDTI                                                     AER21600
  900 CONTINUE                                                          AER21700
      IF(INTRCT) RHOVA=RHOVA+DRHOVA                                     AER21800
C=======================================================================AER21900
C  ALSO UPDATE P AND TAMB IF INTERACTIVE                                AER22000
C   USING TOTAL DELHA AND CONSTANT-VOLUME SPECIFIC HEAT                 AER22100
C=======================================================================AER22200
      IF(RHOVA.LT.0.0) RHOVA=0.0                                        AER22300
```

```
C=======================================================================
C  CALL CONCEN OR NCONCN
C=======================================================================
  950 CALL NCONCN
C
      RETURN
  200 STOP
C=======================================================================
C  FREEZE/MELT LOGIC
C=======================================================================
  300 IF(FROZEN.AND..NOT.TFFLAG) GO TO 370
      IF(.NOT.FROZEN.AND.TFFLAG) GO TO 340
C
      WRITE(1,1010)
 1010 FORMAT(////,25X,10(1H*),8H FROZEN ,10(1H*))
C=======================================================================
C  SET CONSTANTS TO ICE VALUES
C=======================================================================
  310 CLN=CLF
      A=AF
      B=BF
      CSO=CSI
      GO TO 2
C
  340 FROZEN=.TRUE.
      CLN=CLL
      WRITE(1,1020)
 1020 FORMAT(////,25X,10(1H*),18H SWITCH TO FROZEN ,10(1H*))
      IF(.NOT.CWF) GO TO 310
      TLHF=0.0
      DO 350 I=1,NUMPAR
  350 TLHF=TLHF+CN(I)*CM(I)
      TLHF=TLHF*CLN
      WRITE(1,1030) TLHF
 1030 FORMAT(/,10X,16HHEAT RELEASED = ,E11.4)
C=======================================================================
C  UPDATE P AND TAMB IF INTERACTIVE
C=======================================================================
      GO TO 310
C=======================================================================
C  RESET TO LIQUID VALUES
C=======================================================================
  370 FROZEN=.FALSE.
      CLN=CLF
      WRITE(1,1040)
 1040 FORMAT(////,25X,10(1H*),18H SWITCH TO LIQUID ,10(1H*))
      IF(.NOT.CWF) GO TO 1
      TLHF=0.0
      DO 380 I=1,NUMPAR
  380 TLHF=TLHF-CN(I)*CM(I)
      TLHF=TLHF*CLN
C=======================================================================
C  UPDATE P AND TAMB IF INTERACTIVE
C=======================================================================
      WRITE(1,1030) TLHF
      GO TO 1
```

```
C                                                                       AER28000
  400 STOP                                                              AER28100
  500 STOP                                                              AER28200
  700 STOP                                                              AER28300
      END                                                               AER28400
```

```
      SUBROUTINE SETUP
C
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,
     1RHOES,P
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),
     2CF(50,50),DMDT(50),STATE(50),VG(50)
C***********************************************************************
C
C       THE FOLLOWING ARE CONSTANT ASSIGNMENTS  --
C
C***********************************************************************
C
C-----------------------------------------------------------------------
C  CONSTANTS FOR SATURATION VAPOR PRESSURE OVER LIQUID COMPUTATION
      DATA  AL      / 17.27        /
      DATA  BL      / 35.68        /
C-----------------------------------------------------------------------
C  CONSTANTS FOR SATURATION VAPOR PRESSURE OVER ICE COMPUTATION
      DATA  AF      / 21.87        /
      DATA  BF      / 7.66         /
C-----------------------------------------------------------------------
C  BOLTZMANN'S CONSTANT
      DATA  BK      / 1.38E-16     /
C          ERGS / DEGREE KELVIN
C-----------------------------------------------------------------------
C  CONDUCTIVITY OF HEAT IN AIR
      DATA  CK      / 2.42E3       /
C          ERGS / CENTIMETER - SECOND - DEGREE KELVIN
C-----------------------------------------------------------------------
C  LATENT HEAT OF FREEZING OF WATER AT ZERO DEGREES CENTIGRADE
      DATA  CLF     / 2.83E10      /
C          ERGS / GRAM
C-----------------------------------------------------------------------
C  LATENT HEAT OF VAPORIZATION OF WATER AT ZERO DEGREES CENTIGRADE
      DATA  CLL     / 2.5E10       /
C          ERGS / GRAM
C-----------------------------------------------------------------------
C  MOLECULAR WEIGHT OF WATER
      DATA  CMW     / 18.0         /
C-----------------------------------------------------------------------
C  SPECIFIC HEAT OF AIR AT CONSTANT PRESSURE AND TEMPERATURE TAMB
      DATA  CP      / 1.01E7       /
C-----------------------------------------------------------------------
C  SPECIFIC HEAT OF WATER (ICE VALUE)
      DATA  CSI     / 2.09E7       /
C          ERGS / GRAM - DEGREE KELVIN
C-----------------------------------------------------------------------
C  SPECIFIC HEAT OF WATER (LIQUID VALUE)
```

```
      DATA  CSW     / 4.18E07       /                                   SET05600
C           ERGS / GRAM - DEGREE KELVIN                                 SET05700
C-----------------------------------------------------------------------SET05800
C  CONSTANTS FOR COMPUTING VENTILATION FACTOR                           SET05900
      DATA  CVH     / 0.3           /                                   SET06000
      DATA  CVM     / 0.3           /                                   SET06100
C-----------------------------------------------------------------------SET06200
C  STANDARD VALUE FOR DIFFUSIVITY OF WATER                              SET06300
      DATA  DNOT    / .220          /                                   SET06400
C           CENTIMETER   2 / SECOND                                     SET06500
C-----------------------------------------------------------------------SET06600
C  COEFFICIENT OF TETENS EQUATION FOR VAPOR PRESSURE                    SET06700
      DATA  ESO     / 6108.         /                                   SET06800
C-----------------------------------------------------------------------SET06900
C  STANDARD PRESSURE                                                    SET07000
      DATA   PNOT   / 1.013E6       /                                   SET07100
C           DYNES / CENTIMETER   2                                      SET07200
C-----------------------------------------------------------------------SET07300
C  DENSITY OF WATER                                                     SET07400
      DATA  RHOW    / 1.0           /                                   SET07500
C           GRAMS / CENTIMETER   3                                      SET07600
C-----------------------------------------------------------------------SET07700
C  STANDARD TEMPERATURE                                                 SET07800
      DATA  TNOT    / 273.          /                                   SET07900
C           DEGREES KELVIN                                              SET08000
C-----------------------------------------------------------------------SET08100
C  GAS CONSTANT                                                         SET08200
      DATA  RG      / 8.314E7       /                                   SET08300
C           ERGS / MOL - DEGREE KELVIN                                  SET08400
C-----------------------------------------------------------------------SET08500
C  FREEZING TEMPERATURE                                                 SET08600
      DATA  TF      / 273.16        /                                   SET08700
C           DEGREES KELVIN                                              SET08800
C-----------------------------------------------------------------------SET08900
C                                                                       SET09000
C=======================================================================SET09100
C  DIFFUSIVITY OF WATER VAPOR - ICT EQUATION                            SET09200
C=======================================================================SET09300
      D=DNOT*(TAMB/TNOT)**1.81*(PNOT/P)                                 SET09400
C                                                                       SET09500
      NUM1=NUMPAR.EQ.1                                                  SET09600
      NUM2=NUMPAR.EQ.2                                                  SET09700
      CLM=CLF-CLL                                                       SET09800
      PI=4.0*ATAN(1.0)                                                  SET09900
      IF(NUM1) GO TO 60                                                 SET10000
      DO 50 I=2,NUMPAR                                                  SET10100
      DIFCM(I-1)=CM(I)-CM(I-1)                                          SET10200
   50 CONTINUE                                                          SET10300
   60 DIFCM(NUMPAR)=1.0                                                 SET10400
      RETURN                                                            SET10500
      END                                                               SET10600
```

```
      SUBROUTINE COLLIS
C
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,
     1RHOES,P
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),
     2CF(50,50),DMDT(50),STATE(50),VG(50)
      DIMENSION DB(50)
C=======================================================================
C  VISCOSITY OF AIR - SUTHERLAND EQUATION - CGS UNITS
C=======================================================================
      VISC=TAMB**1.5*145.8E-07/(110.4+TAMB)
C
C=======================================================================
C  COMPUTE BROWNIAN COLLISION FREQUENCY FB
C=======================================================================
      TEMPD=BK*TAMB/(6.0*PI*VISC)
      DO 100 I=1,NUMPAR
      DB(I)=TEMPD/RAD(I)
  100 CONTINUE
      DO 300 J=1,NUMPAR
      DO 200 I=1,NUMPAR
      RIJ=RAD(I)+RAD(J)
      FB=4.0*(DB(I)+DB(J))
C
C=======================================================================
C  ADD GRAVITATIONAL COLLISION FREQUENCY FGT
C=======================================================================
      CF(I,J)=FB+FGT(I,J)
C
  200 CONTINUE
  300 CONTINUE
      WRITE(1,1000)VISC
 1000 FORMAT(/,35X,12HVISCOSITY = ,E10.4)
      RETURN
      END
```

```
      FUNCTION FGT(I,J)                                                 FGT00000
C                                                                       FGT00100
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,  FGT00200
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM                            FGT00300
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,       FGT00400
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP                                   FGT00500
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,         FGT00600
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,                  FGT00700
     2SPEMIN,GK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO                   FGT00800
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,                    FGT00900
     1RHOES,P                                                           FGT01000
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),          FGT01100
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),                       FGT01200
     2CF(50,50),DMDT(50),STATE(50),VG(50)                               FGT01300
      FGT=0.0                                                           FGT01400
C=======================================================================FGT01500
C  DUMMY VALUE OF FGT WHEN V(I) AVAILABLE REPLACE BY                    FGT01600
C    RIJ = RAD(I) + RAD(J)                                              FGT01700
C    FGT = PI * RIJ * RIJ * ABS(V(I) - V(J))                            FGT01800
C     OR USE FALLING RATES VG INSTEAD OF V                              FGT01900
C=======================================================================FGT02000
      RETURN                                                            FGT02100
      END                                                               FGT02200
```

```
      SUBROUTINE NCONCN
C
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,
     1RG,RHOW,ONETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,
     1RHOES,P
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),
     2CF(50,50),DMDT(50),STATE(50),VG(50)
      DIMENSION TN(50)
      LOGICAL NSPMFG
      IF(NAGLOM) GO TO 50
      CALL COLLIS
   50 NSPMFG=S.LT.SPEMIN
      WRITE(1,1000)
 1000 FORMAT(//,76X,7HRATE OF,
     1/,30X,5HCLASS,5X,23HCHANGE IN CONCENTRATION,5X,
     223HCHANGE IN CONCENTRATION,/,42X,18HDUE TO EVAPORATION,11X,
     320HDUE TO AGGLOMERATION,/,44X,15HOR CONDENSATION,/,30X,5H-----,
     45X,23(1H-),5X,23(1H-))
C=======================================================================
C  COMPUTE CHANGE OF CLASS 1
C=======================================================================
      CNI1=CN(1)
      DNDTAG=0.0
      IF(NAGLOM) GO TO 104
      DO 100 J=1,NUMPAR
  100 DNDTAG=DNDTAG-CF(1,J)*CN(J)
      IF(TFIX) GO TO 103
C=======================================================================
C  TO PERMIT VARIABLE DELTIM WITH '.SKIP.', REVISE
C    AEROSOL TO COMPUTE DELHA AND DRHOVA AFTER
C    CALL OF NCONCN
C=======================================================================
  101 IF(SKIP.OR.DNDTAG*DELTIM.LE.C) GO TO 102
      DELTIM=DELTIM/2.
      GO TO 101
  102 IF(SKIP.OR.DNDTAG*DELTIM.GE.C/2.) GO TO 103
      DELTIM=DELTIM*2.
      GO TO 102
  103 DNDTAG=DNDTAG*CNI1
      IF(SKIP) GO TO 104
      DELCNI=0.0
      GO TO 105
  104 IF(DELCM(1).GT.0.0) DELCNI=-CNI1*DELCM(1)/DIFCM(1)+AMAX1(0.0,
     1-CN(2)*DELCM(2)/DIFCM(1))
C=======================================================================
C  CLASS 1 CANNOT LOSE MASS TO SMALLER PARTICLES
C=======================================================================
      IF(DELCM(1).LE.0.0) DELCNI=AMAX1(0.0,
     1-CN(2)*DELCM(2)/DIFCM(1))
```

```
  105 TN(1)=CNI1+DNDTAG*DELTIM+DELCNI                                   NC005600
      I=1                                                               NC005700
      WRITE(1,1200) I,DELCNI,DNDTAG                                     NC005800
 1200 FORMAT(30X,I3,10X,E12.4,11X,E12.4)                                NC005900
C                                                                       NC006000
      IF(NUM1) GO TO 205                                                NC006100
C=======================================================================NC006200
C  COMPUTE CHANGE OF CLASS 2                                            NC006300
C=======================================================================NC006400
      CNI=CN(2)                                                         NC006500
      DNDTAG=0.0                                                        NC006600
      IF(NAGLOM) GO TO 113                                              NC006700
      DNDTAG=-CF(2,1)*CNI1*.5                                           NC006800
      DO 110 J=2,NUMPAR                                                 NC006900
  110 DNDTAG=DNDTAG-CF(2,J)*CN(J)                                       NC007000
      DNDTAG=DNDTAG*CNI+CF(1,1)*CNI1*CNI1*.5                            NC007100
      IF(SKIP) GO TO 113                                                NC007200
      DELCNI=0.0                                                        NC007300
      GO TO 115                                                         NC007400
  113 IF(DELCM(2).GT.0.0) DELCNI=-CNI*DELCM(2)/DIFCM(2)+AMAX1(0.0,      NC007500
     1CN(1)*DELCM(1)/DIFCM(1))+AMAX1(0.0,-CN(3)*DELCM(3)/DIFCM(2))      NC007600
      IF(DELCM(2).LE.0.0) DELCNI=CNI*DELCM(2)/DIFCM(1)+AMAX1(0.0,       NC007700
     1CN(1)*DELCM(1)/DIFCM(1))+AMAX1(0.0,-CN(3)*DELCM(3)/DIFCM(2))      NC007800
  115 TN(2)=CNI+DNDTAG*DELTIM+DELCNI                                    NC007900
      I=2                                                               NC008000
      WRITE(1,1200) I,DELCNI,DNDTAG                                     NC008100
C                                                                       NC008200
      IF(NUM2) GO TO 205                                                NC008300
C=======================================================================NC008400
C  COMPUTE CHANGE OF CLASSES 3 THROUGH NUMPAR                           NC008500
C=======================================================================NC008600
      DO 200 I=3,NUMPAR                                                 NC008700
      CNI1=CNI                                                          NC008800
      CNI=CN(I)                                                         NC008900
      AGLOM1=0.0                                                        NC009000
      AGLOM2=0.0                                                        NC009100
      DNDTAG=0.0                                                        NC009200
      I1=I-1                                                            NC009300
      I2=I-2                                                            NC009400
      IF(NAGLOM) GO TO 131                                              NC009500
      DO 120 J=I,NUMPAR                                                 NC009600
  120 DNDTAG=DNDTAG-CF(I,J)*CN(J)                                       NC009700
      TWOJI=2.0**(1-I)                                                  NC009800
      DO 130 J=1,I2                                                     NC009900
      AGLOM1=AGLOM1-CF(I,J)*CN(J)*TWOJI                                 NC010000
      TWOJI=TWOJI*2.0                                                   NC010100
      AGLOM2=AGLOM2+CF(I1,J)*TWOJI*CN(J)                                NC010200
  130 CONTINUE                                                          NC010300
      AGLOM1=AGLOM1-CF(I,I1)*CN(I1)*.5                                  NC010400
      AGLOM2=AGLOM2+CF(I1,I1)*.5*CNI1                                   NC010500
      DNDTAG=(DNDTAG+AGLOM1)*CNI+AGLOM2*CNI1                            NC010600
      IF(SKIP) GO TO 131                                                NC010700
      DELCNI=0.0                                                        NC010800
      GO TO 135                                                         NC010900
  131 IF(I.LT.NUMPAR) GO TO 133                                         NC011000
      DELCNI=AMAX1(0.0,CN(I1)*DELCM(I1)/DIFCM(I1))                      NC011100
```

```
      GO TO 135                                                         NC011200
  133 IF(DELCM(I).GT.0.0) DELCNI=-CN(I)*DELCM(I)/DIFCM(I)+AMAX1(0.0,    NC011300
     1CN(I1)*DELCM(I1)/DIFCM(I1))+                                      NC011400
     2AMAX1(0.0,-CN(I+1)*DELCM(I+1)/DIFCM(I))                           NC011500
      IF(DELCM(I).LE.0.0) DELCNI=CN(I)*DELCM(I)/DIFCM(I)+AMAX1(0.0,     NC011600
     1CN(I1)*DELCM(I1)/DIFCM(I1))+                                      NC011700
     2AMAX1(0.0,-CN(I+1)*DELCM(I+1)/DIFCM(I))                           NC011800
  135 TN(I)=CNI+DNDTAG*DELTIM+DELCNI                                    NC011900
      WRITE(1,1200) I,DELCNI,DNDTAG                                     NC012000
  200 CONTINUE                                                          NC012100
C                                                                       NC012200
C=======================================================================NC012300
C  UPDATE ALL CN                                                        NC012400
C=======================================================================NC012500
  205 DO 210 I=1,NUMPAR                                                 NC012600
  210 CN(I)=TN(I)                                                       NC012700
C                                                                       NC012800
C=======================================================================NC012900
C  TEST FOR APPEARANCE/DISAPPEARANCE OF CONDENSED WATER                 NC013000
C=======================================================================NC013100
      IF(CWF) GO TO 160                                                 NC013200
C=======================================================================NC013300
C  CLASS 1 PARTICLES TREATED AS DRY NUCLEI                              NC013400
C=======================================================================NC013500
      IF(NSPMFG) RETURN                                                 NC013600
      IF(DELCM.GT.0.0) GO TO 150                                        NC013700
  140 CONTINUE                                                          NC013800
      RETURN                                                            NC013900
  150 CWF=.TRUE.                                                        NC014000
      RETURN                                                            NC014100
  160 DO 170 I=2,NUMPAR                                                 NC014200
      IF(CN(I).GT.0.0) RETURN                                           NC014300
  170 CONTINUE                                                          NC014400
C                                                                       NC014500
      IF(NSPMFG) CWF=.FALSE.                                            NC014600
      RETURN                                                            NC014700
      END                                                               NC014800
```

```
      SUBROUTINE CONCEN
C
C=======================================================================
C  WARNING -- CONCEN MAY ONLY BE VALID FOR
C    CONDENSING NOT EVAPORATING PARTICLES
C=======================================================================
C
      COMMON/FLAGS/FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP,INSTFM
      LOGICAL FIRST,IMPURE,INTRCT,INSTCN,FROZEN,PSMALL,NUM1,NUM2,
     1TFIX,VFSIG,CDHC,CWF,NAGLOM,SKIP
      COMMON/CONSTN/C,CK,CLF,CLL,CM(50),CMW,CSW,D,DELTIN,HL,PI,
     1RG,RHOW,UNETRD,CVM,CVH,DIFCM(50),NUMPAR,RHOP,CP,
     2SPEMIN,BK,TNOT,PNOT,DNOT,AF,BF,TF,AL,BL,CSI,ESO
      COMMON/VARIAB/DELTIM,RHOVA,TAMB,TIM,CNU,S,A,B,
     1RHOES,P
      COMMON/ARRAYS/CN(50),CSD(50),DELHA(50),DELWV(50),HD(50),
     1RHOVS(50),RAD(50),TSUR(50),V(50),DELCM(50),
     2CF(50,50),DMDT(50),STATE(50),VG(50)
      DIMENSION DN(50)
      LOGICAL SPEMFG
      IF(NAGLOM) GO TO 50
      CALL CELLIS
      WRITE(1,1000)
 1000 FORMAT(//,48X,7HRATE OF,
     1/,30X,5HCLASS,5X,23HCHANGE IN CONCENTRATION,
     2/,41X,20HDUE TO AGGLOMERATION,/,30X,5H-----,
     35X,23(1H-))
   50 NSPMFG=S.LT.SPEMIN
C  COMPUTE CHANGE OF CLASS 1
      CNI2=CN(1)
      DNDTAG=0.
      IF(NAGLOM) GO TO 102
      DO 90  J=1,NUMPAR
      DNDTAG=DNDTAG+CF(1,J)*CN(J)
   90 CONTINUE
   92 IF(TFIX) GO TO 97
      IF(SKIP.OR.DNDTAG*DELTIM.LE.0) GO TO 97
C=======================================================================
C  TO PERMIT VARIABLE DELTIM WITH '.SKIP.', REVISE
C    AEROSOL TO COMPUTE DELHA AND DRHOVA AFTER
C    CALL OF CONCEN
C=======================================================================
      DELTIM=DELTIM/2.
      GO TO 92
   97 IF(SKIP) GO TO 102
      DN(1)=-CNI2*DNDTAG
      GO TO 103
  102 DN(1)=-CNI2*DMDT(1)/DIFCM(1)-CNI2*DNDTAG
C
  103 IF(NUM1) GO TO 125
      CNI1=CN(2)
C=======================================================================
C  XDND IS RATE OF CHANGE OF CN(1) DUE TO AGGLOMERATION
C=======================================================================
      XDND=-CNI2*DNDTAG
```

```
      IJK=1
      WRITE(1,1100) IJK,XDND
 1100 FORMAT(30X,I3,10X,E12.4)
C=======================================================================
C  COMPUTE CHANGE OF CLASS 2
C=======================================================================
      DNDTAG=0.
      IF(NAGLOM) GO TO 106
      DO 105 J=1,NUMPAR
      DNDTAG=DNDTAG+CF(2,J)*CN(J)
  105 CONTINUE
C=======================================================================
C  XDND IS RATE OF CHANGE OF CN(2) DUE TO AGGLOMERATION
C=======================================================================
      XDND=-CNI1*DNDTAG+.5*CF(1,1)*CNI2*CNI2
      IJK=2
      WRITE(1,1100) IJK,XDND
      IF(SKIP) GO TO 106
      DN(2)=-CNI1*DNDTAG+.5*CF(1,1)*CNI2*CNI2
      GO TO 107
  106 DN(2)=-CNI1*DMDT(2)/DIFCM(2)+CNI2*DMDT(1)/DIFCM(1)-CNI1*DNDTAG
     1 +.5*CF(1,1)*CNI2*CNI2
  107 IF(NUM2) GO TO 125
C=======================================================================
C  COMPUTE CHANGE OF CLASSES 3 THROUGH NUMPAR
C=======================================================================
      DO 120 I=3,NUMPAR
      CNI=CN(I)
      IF(I.EQ.NUMPAR) CNI=0.0
      I1=I-1
      I2=I-2
      IF(SKIP) GO TO 108
      DNDTEC=0.0
      GO TO 109
  108 DNDTEC=CNI1*DMDT(I1)/DIFCM(I1)-CNI*DMDT(I)/DIFCM(I)
      DNTDAG=0.0
      IF(NAGLOM) GO TO 117
  109 DNDTAG=.5*CF(I1,I1)*CNI1*CNI1+.75*CF(I1,I2)*CNI1*CNI2
      SUMA=0.0
      TWOJ1=2.0**(1-I)
      DO 110 J=1,I2
      SUMA=SUMA+CF(I,J)*CN(J)*TWOJ1
      TWOJ1=TWOJ1*2.
  110 CONTINUE
      SUMB=0.0
      DO 115 J=I1,NUMPAR
      SUMB=SUMB+CF(I,J)*CN(J)
  115 CONTINUE
      IF(I.EQ.NUMPAR) CNI=CN(I)
      DNDTAG=DNDTAG+CNI*(SUMA-SUMB)
C=======================================================================
C  DN IS TOTAL RATE OF CHANGE OF CN
C=======================================================================
  117 DN(I)=DNDTEC+DNDTAG
      CNI2=CNI1
      CNI1=CNI
```

```
      WRITE(1,1100) I,DMPTAG                                            CON11200
  120 CONTINUE                                                          CON11300
C=======================================================================CON11400
C  UPDATE ALL CN                                                        CON11500
C=======================================================================CON11600
  125 DO 130  I=1,NUMPAR                                                CON11700
  130 CN(I)=CN(I)+DN(I)*DELTIM                                          CON11800
C                                                                       CON11900
C=======================================================================CON12000
C  TEST FOR APPEARANCE/DISAPPEARANCE OF CONDENSED WATER                 CON12100
C=======================================================================CON12200
      IF(CWF) GO TO 160                                                 CON12300
      IF(NSPMFG) RETURN                                                 CON12400
      DO 140  I=1,NUMPAR                                                CON12500
      IF(DELCM(I).GT.0.0) GO TO 150                                     CON12600
  140 CONTINUE                                                          CON12700
      RETURN                                                            CON12800
  150 CWF=.TRUE.                                                        CON12900
      RETURN                                                            CON13000
  160 DO 170  I=2,NUMPAR                                                CON13100
      IF(CN(I).GT.0.0) RETURN                                           CON13200
  170 CONTINUE                                                          CON13300
C                                                                       CON13400
      IF(NSPMFG) CWF=.FALSE.                                            CON13500
      RETURN                                                            CON13600
      END                                                               CON13700
```

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