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QUICK Users' Manual

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ABSTRACT

The QUICK reference computer code for singly contained, single component, aerosol behavior is described. The model equation used is presented and the numerical solution technique -- modified finite difference coupled with the GEAR ordinary differential equation solver -- is discussed briefly. A short description of each subroutine is presented and the logic of the code described in a flow diagram. Input required by QUICK is given in detail, as is the result of a sample run. QUICK is intended to provide a best estimate of aerosol behavior in a homogeneously mixed, nonflowing containment atmosphere. The aerosol particles are assumed to be characterizable by a constant material density, particle mass, a constant dynamic shape factor and a constant collision form factor.

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INTRODUCTION

The behavior of aerosols in reactor containments represents an important link in the causal chain of radioactivity transport from its source in a disrupted core to the environment. For this reason, research into the behavior of enclosed aerosols has been in progress for a number of years and has resulted in several aerosol behavior codes.

The QUICK code is the latest result of an extended research program under U.S. NRC auspices into numerical methods for solving the one component aerosol behavior problem in as rigorous a fashion as possible. A comparison of several candidate methods has suggested that the relatively straightforward numerical approach employed by QUICK yields results that are negligibly different than those of more sophisticated methods[1] and does so with the advantage of much shorter computation times. QUICK was therefore chosen as a reference standard and its capabilities in terms of types of input and output and included behavior mechanisms enhanced to the level of codes, such as HARM-3[2], that are in routine use.

In the following, the mathematical formulation of the model and a brief description of the numerical approach to its solution are given. Following this, brief descriptions of the subroutines and input parameters of the code are given. Finally, a test case with both input and output is presented.

MODEL EQUATIONS

The underlying assumption of the model equations, one that is made by most present aerosol behavior codes, is that the aerosol can be viewed as a homogeneous mixture, except for narrow surface boundary layers through which mass transport of the particulate phase takes place. This assumption was tested for the special case of sodium pool fire aerosols with a model[3] that

sub-compartmentalizes the containment into three individually mixed zones connected by fluid flow and found to be adequate after the fire ceases and conservative during the burn period. It permits model equations that are independent of spatial coordinates and thus makes their numerical solution practicable.

The second, fundamental assumption is that the expected non-sphericicity and fluffiness of the aerosol agglomerates can be modeled using just two size independent correction factors -- the dynamic shape factor and the collision shape factor. These will be treated below. Their size independence is not an inherent requirement of the code but a convenient assumption in lieu of experimental data to the contrary.

Given these assumptions, the general equation of aerosol behavior is:

$$\frac{\partial n(x,t)}{\partial t} = S(x,t) - R(x,t)n(x,t) - L(x,t)n(x,t) - F(x,t)n(x,t) + \frac{1}{2}\int_0^x K(x',x-x')n(x',t)n(x-x',t)dx' - n(x,t)\int_0^\infty K(x,x')n(x',t)dx' \quad (1)$$

Here

$n(x,t)dx$ = number of particles of mass x in dx at time t per unit volume

$S(x,t)dx$ = number of particles of mass x in dx uniformly introduced into the aerosol system per unit time per unit volume

$R(x,t)n(x,t)dx$ = number of particles of mass x in dx uniformly removed from the aerosol system per unit time per unit volume by deposition

$L(x,t)n(x,t)dx$ = number of particles of mass x in dx uniformly removed from the aerosol system per unit time per unit volume by leaks

$F(x,t)n(x,t)dx$ = number of particles of mass x in dx uniformly removed from the aerosol system per unit time per unit volume by filters

$K(x,x')n(x)n(x')dxdx'$ = number of collisions between particles of mass x in dx and x' in dx' per unit time per unit volume.

Source Term

This term can be an arbitrary function of time. For convenience, the particle number size distribution density is assumed to be lognormal, but with arbitrary time dependence of the total number, geometric mean radius and logarithmic standard deviation.

Natural Removal Terms

Natural removal by sedimentation diffusion and thermophoresis are considered. This is described in general by a deposition velocity, $v(x,t)$, such that

$$R(x,t) = v(x,t)\frac{A_i}{V} \tag{2}$$

where

A_i = surface area available for deposition due to mechanism i

V = volume of containment.

v is taken as the steady state velocity $v = B(x)\cdot F(x,t)$ with $B(x)$ the mobility of a particle of mass x and $F(x,t)$ the applied force. The mobility is given by

$$B(x) = \frac{1}{\chi 6\pi\mu r_e}\left(1+AKn+QKne^{-b/Kn}\right) \tag{3}$$

with

χ = dynamic shape factor

μ = viscosity of gas

$r_e = \left(\frac{3x}{4\pi\rho_p}\right)^{1/3}$

ρ_p = particle material density

Kn = Knudsen number of particle

$A = 1.246$, $Q = 0.42$, $b = 0.87$.

Here the Knudsen-Weber-Cunningham correction constants are those of Millikan for oil drops[4]. Their precise values depend on the particle constituents but do not enter sensitively into typical code predictions.

(i) Sedimentation

For particle Reynold's numbers less than one, the Stoke's settling velocity

$$v(xt) = \frac{4\pi}{3} r_e^3 \rho_p g \, B(x) \qquad (4)$$

holds. For some severe accident scenarios, however, QUICK predicts a large fraction of the suspended mass to reside in particles whose diameter exceeds 100 μm. For these, Equation (4) no longer holds and may in fact be off by as much as a factor of two. QUICK therefore uses empirical data[5] in the form of a correction factor to expression (4) for particles whose Reynold's number is greater than one and less than 1259. For Reynold's numbers in excess of this value, no empirical values of v are known. As a compromise, the correction value for $R_e = 1259$ is used here as well.

To account for particle nonsphericity, it is assumed that a correction factor, f, exists such that

$$fC_F = \frac{F_D}{\pi r_e^2 \gamma^2 \frac{\rho_g}{2} v^2}$$

where γ = collision shape factor

C_F = Fanning friction factor for spheres

F_D = actual drag force on particle

From the limit requirement that

$$F_D = 6\pi\mu x r_e v$$

and

$$v = \frac{2}{9} \frac{\rho_p g r_e^2}{\mu x}$$

in the Stoke's regime, one can determine f to be equal to x/γ.

The collision shape factor, γ, was initially introduced[6] to account for a collision cross-section of nonspherical particles that depends on a collision radius, r_c, different than r_e. Thus r_c was taken as proportional to r_e: $r_c = \gamma r_e$. γ has never been measured, but approximate values have been inferred by backfitting computer codes. Unfortunately, γ has also been shown, along with χ, to be the most sensitive code parameter.[7]

To avoid the introduction of further parameters of comparable sensitivity, γ is also used in QUICK as a proportionality factor between some geometric particle radius, r, of an agglomerated, nonspherical, particle and its mass equivalent radius: $r = \gamma r_e$. Then all data correlated on spherical particles is written in terms of γr_e. Thus, in particular, $Kn \equiv \lambda/\gamma r_e$, where λ is the gas phase mean free path.

(ii) Diffusion

$$v(xt) = \frac{D(x)}{\delta_D} \tag{5}$$

where

$D(x) = B(x)kT$

k = Boltzmann's constant

T = absolute temperature

δ_D = diffusion boundary layer thickness.

δ_D is known to depend on the momentum boundary layer thickness, δ_o, of the flowing gas-wall interface and on particle size through its dependence on D(x) via

$$\delta_D \equiv \delta_o \, Sc^{-1/3}$$

where

$Sc = \frac{\mu}{\rho_g D}$ = Schmidt number

ρ_g = density of gas phase.

Nevertheless, δ_D is assumed an input constant since experimental evidence to the contrary is scarce and, more importantly, since diffusive deposition appears to play a minor role in reactor accident calculations.

(iii) Thermophoresis

Thermophoresis is driven by temperature gradients. These are usually not well known everywhere so that considerable uncertainty in code output exists for cases in which thermophoresis is significant. Because of this uncertainty, great precision in the expression for the thermophoretic deposition velocity is not necessary. The code uses an expression, developed by Brock[8], that agrees within a factor of two with available data:

$$F_{thermophoresis} = \frac{-9\pi\mu^2 r_e \gamma}{\rho_p} \phi \frac{\Delta T}{T\delta_{TH}} \qquad (6)$$

where

$$\phi = \left(\frac{1}{1+3C_m Kn}\right)\left(\frac{\frac{k_g}{k_p} + C_t Kn}{1+\frac{2k_g}{k_p} + 2C_t Kn}\right)$$

ΔT = temperature difference between wall surface and gas over the thermal boundary layer thickness, δ_{TH}.

C_m = momentum accommodation coefficient, taken as 1.0.

C_t = thermal accommodation coefficient, taken as 2.49.

k_g = thermal conductivity of the gas phase.

k_p = thermal conductivity of a particle.

Since the Brock expression for the thermophoretic force is based on spherical particles, γr_e is used wherever a particle radius is referenced.

The values of C_m and C_t indicated are those that result in the best fit of expression (6) with data or NaCl aerosol.[9] Measurements on dry Na_2O_2 particles[10] have yielded values of C_t between 1.9 and 2.5, with the former value based on the assumption that $k_g/k_p = 0.01$, the latter on kg/kp = 1.0. For fluffy agglomerates, the thermal conductivity, k_p, as used in expression (6) probably does not correspond to the particle's material thermal conductivity. It is likely that k_p approaches k_g with increasing fluffiness, but no independent measurements of k_p are known.

It should be noted that for severe accident scenarios, most of the airborne mass is associated with particles whose Knudsen number is small. In this case,

$$\phi \rightarrow \frac{1}{2+k_p/k_g} \quad ,$$

and is thus essentially independent of C_t, C_m, but a strong function of the unknown, k_p. Its uncertainty is comparable, in effect, to that in the average thermal gradient at interior surfaces.

Leakage

Aerosol particles can be removed from the system by a time dependent leak that has an associated particle capture efficiency, $\varepsilon_L(x)$.

$$L(x,t) = \frac{\dot{V}_L}{V} \tag{7}$$

where

$\dot{V}_L$ = volumetric gas leak rate.

The source rate of aerosol number to the environment is

$$[1-\varepsilon_L(x)]n(x,t)dx \tag{8}$$

Recirculating Filtration

Again, a size dependent filtration efficiency, $\varepsilon_F(x)$ is permitted such that

$$F(x,t) = \varepsilon_F(x) \frac{\dot{V}_F}{V}$$

where

$\dot{V}_F$ = volumetric filtration throughput.

Coagulation

Of the multitude of mechanisms that can contribute to particle collisions (and therefore coagulation) only two appear to play a significant role in passive aerosol systems: Brownian and gravitational coagulation. The QUICK code includes these and turbulent coagulation since the latter may play a role in situations where natural convection due to large scale fires becomes severe enough to result in significant turbulent energy dissipation. Turbulent coagulation has not, however, appeared to have played a significant role in the largest sodium fire simulation experiments to date.

(i) Brownian Coagulation

$$K(x,x') = \pi kT\gamma[B(x)+B(x')](r_e+r_e') \tag{9}$$

(ii) Gravitational Coagulation

$$K_G(x,x') = \varepsilon(x,x') \frac{2\pi g \rho_p \gamma^2}{9\mu\chi} \left| r_e^2 - r_e'^2 \right| (r_e+r_e')^2 \tag{10}$$

where

$\varepsilon(x,x')$ = collision efficiency.

The collision efficiency can be viewed as that factor which makes expression (1) correct. Most recent experimental and theoretical investigations into this factor (11) have yielded data tables that have been employed in QUICK on large scale sodium fire simulation runs. The results of these runs are surprisingly similar to ones using the simple expression

$$\varepsilon(x,x') = 1.5 \left(\frac{r}{r+r'}\right)^2 \tag{11}$$

where x', (r') refer to the larger particle. Expression (11) strictly holds for inertialess particles and r'>>r only. Its use for all values of r' and r yields satisfactory agreement with simulation experiments to date.

Turbulent Coagulation

An expression for turbulent coagulation was added to QUICK in the expectation that severe sodium fires would lead to sufficient turbulence production to make this mechanism significant. Present simulation experiments suggest that it plays a noticeable, but minor, role.

The two most widely used theoretical treatments of turbulent coagulation are probably those of Saffman and Turner[12] and Levich[13]. Both are based on the hypothesis that microscale turbulence is essentially isotropic and that the particles are smaller than the microscale. Both also invoke the same conceptualization of the turbulent collision process: relative particle motion due to entrainment in a variable fluid velocity field and relative particle motion due to differences in inertial response to fluid acceleration. It is not surprising therefore that, since quantification of isotropic microscale turbulence is based on dimensional analysis, the two approaches result in identical expressions except for multiplicative constants. By the same token, these multiplicative constants must be considered indeterminate until experimentally determined.

The QUICK expression for turbulent coagulation is based on Saffman and Turner's, including their multiplicative constants. Their expressions have been modified to include a collision efficiency for particle motion relative to the fluid and the shape factors for non-spherical particles discussed above. While the collision efficiency for particles colliding due to their motion with a variable fluid velocity field may not be unity, no ansatz is known for its treatment and none is made in QUICK. Thus

$$K_{T+G}(x,x') = 2\sqrt{2\pi}\,\gamma^2(r_e+r_e')^2\left[\varepsilon(x,x')^2(\tau_1-\tau_2)^2\,\frac{1.3E}{\nu}^{3/2}\right. \qquad (12)$$
$$\left. + \frac{1}{3}\,\varepsilon(x,x')^2\,(\tau_1-\tau_2)^2 g^2 + \frac{1}{9}\,\gamma^2(r_e+r_e')^2\,\frac{E}{\nu}\right]^{1/2}$$

where

$\tau = \dfrac{2r_e^{\,2}\rho_p}{9\chi\mu}$ = particle response time

ν = kinematic viscosity of the gas

E = turbulent dissipation energy density.

Note that, following Saffman and Turner, the gravitational coagulation mechanism is incorporated into K_{T+G}.

Finally, the assumption is made that

$$K(x,x') = K_B(x,x') + K_{T+G}(x,x') \quad . \tag{13}$$

Since K_B and K_{T+G} are of equal magnitude over a narrow particle size range only, this approach is not expected to result in significant error.

NUMERICAL METHOD

For numerical reasons, as well as to provide the tools for rigorous scaling of experimental results to full scale containments, Equation (1) is nondimensionalized before being treated by QUICK. The normalizing dimensions used are:

The characteristic time for Brownian coagulation:

$$\tau_{BC} = \frac{1}{K_o N_o} \tag{14}$$

where

$$K_o \equiv \frac{2kT\gamma}{3\mu\chi}$$

N_o = initial total particle number concentration.

= SNR × t_s in the case of no initial aerosol

SNR = average particle number concentration source rate

t_s = duration of source.

and the characteristic initial or source particle size:

$$r_o = \left(\frac{3x_o}{4\pi\rho_p}\right)^{1/3} \tag{15}$$

where

x_o = average initial or source aerosol particle mass

With these, Equation (1) is converted to a nondimensional equation that depends on dimensional parameters only through the nondimensional groups that appear as multiplicative factors, one for each mechanism (except Brownian coagulation). The nondimensional groups are:

(i) Source

$$SRBC = (K_o N_o t_x)^{-1} \tag{16}$$

(ii) Sedimentation

$$GDBC = v_o \frac{A_s}{V} \frac{1}{K_o N_o} \tag{17}$$

where

$$v_o = \frac{2\rho_p g r_o^2}{9\chi\mu}$$

A_s = surface area available for sedimentation.

(iii) Diffusion

$$DDGD = \frac{kT}{\delta_D g x_o} \frac{A_d}{A_s} \tag{18}$$

where

A_d = surface area available for diffusion.

(iv) Thermophoresis

$$THGD = \frac{27}{4} \frac{\mu^2 \gamma}{\rho_g \rho_p g r_o^2} \frac{\Delta T_o}{T} \frac{1}{\delta_{TH}} \frac{A_{TH}}{A_s} \tag{19}$$

where

A_{TH} = surface area available for thermophoretic deposition.

ΔT_o = characteristic temperature difference, wall-gas, over area A_{TH}.

(v) Leakage

$$VLGD = \frac{\dot{V}_L}{V} \frac{1}{K_o N_o} \frac{1}{GDBC} \tag{20}$$

(vi) Filtration

$$VFGD = \frac{\dot{V}_F}{V} \frac{1}{K_o N_o} \frac{1}{GDBL} \tag{21}$$

(vii) Gravitational Coagulation

$$GCBC = \frac{\gamma^2 \pi r_o^2 v_o}{K_o} \tag{22}$$

(viii) Turbulent Coagulation

Motion with fluid

$$TCBC1 = \frac{1}{3} \frac{\gamma^3 r_o^3 E}{K_o \nu^{1/2}}^{1/2}$$

Motion relative to fluid

$$TCBC2 = \frac{1.14 \gamma^2 r_o^2 \tau_o E}{K_o \nu^{1/4}}^{3/4} \tag{24}$$

where

$$\tau_o = v_o/g$$

These eight groups suffice to completely determine the aerosol model QUICK, once initial conditions are set. They can therefore be used in scaling full scale accident scenarios to experimental scale and vice-versa, provided the aerosol aspects of the scenario are amenable to treatment by a one component model.

The numerical approach of QUICK is in essence a straightforward discretization of the nondimensional number distribution on nondimensional particle mass. The resultant system of ordinary differential equations is then solved using the GEAR[14] differential equation solver.

The initial (source) particle size distribution is discretized into a histogram representation by the approximation

$$\tilde{N}_i \equiv \tilde{n}(\tilde{x}'_i,o)\ \Delta\tilde{x}_i \tag{25}$$

where the tildes indicate nondimensionality and

$$\Delta\tilde{x}_i = \tilde{x}_{i+1} - \tilde{x}_i$$

with $\tilde{n}(\tilde{x}'_i,o)$ the value of the distribution density at the geometric mean mass of the interval:

$$\tilde{x}'_i = \left(\tilde{x}_{i+1}\ \tilde{x}_i\right)^{1/2}$$

Nodal spacing is arbitrary.

The model equation, Equation (1), is then reinterpreted in terms of the discrete set, N_i. For the source and removal terms this presents no problem since

$$\tilde{R}(\tilde{x}'_i)\ \tilde{n}(\tilde{x}'_i,t)\ \Delta\tilde{x}_i \rightarrow \tilde{R}(\tilde{x},t)\ \tilde{n}(\tilde{x},t)d\tilde{x}$$

in the limit. The reinterpretation of the collision integrals is, however, more difficult.

Instead of devising a formal discretization scheme of the collision integrals as exhibited in Equation (1), this differential equation is abandoned in favor of a more intuitive picture whose justification lies in the fact that it produces results that closely match those of more rigorous schemes.[1]

In the QUICK code scheme, all particles of an interval are treated identically with characteristics corresponding to the geometric mean mass of the interval defining nodal masses. QUICK then looks at all possible collisions between these representative "particles".

The collision frequency of such collisions is assumed proportional to

$$\tilde{K}(\tilde{x}'_i,\tilde{x}'_j)N_iN_j$$

in anology to the continuum model, Equation (1).

For nodal spacing that increases monotonically, it is easy to show that the collision products of any two collision intervals can at most fall into three consecutive intervals. For a nodal grid that is equi-spaced on the logarithm of the mass (QUICK is set up conveniently for such a grid), only two consecutive intervals are covered by the collision products. In that case the requirements of mass conservation and number accounting uniquely determine the distribution factor, P, such that collisions between intervals $[x_i,x_{i+1}]$ and $[x_j,x_{j+1}]$ create particles in interval $[x_\ell,x_{\ell+1}]$ at the rate $P\tilde{K}(\tilde{x}'_i,\tilde{x}'_j)\tilde{N}_i\tilde{N}_j$ and particles in the interval $[x_{\ell+1},x_{\ell+2}]$ at the rate $[1-P]\tilde{K}(\tilde{x}'_i,\tilde{x}_j)\tilde{N}_i\tilde{N}_j$. Here $P = (\tilde{x}'_\ell-\tilde{x}'_i-\tilde{x}'_j)/(\tilde{x}'_{\ell+1}-\tilde{x}'_\ell)$. It is clear that this scheme reduces to the continuum equation in the limit of infinitesimal noda' spacing. Its adequacy for finite spacing has been tested by comparing widel differing grid arrangements.

Particles that grow beyond the maximum size permitted by the grid system chosen by the user, are collected in a bin and their mass assessed, to ensure conservation of mass in the calculations. This scheme also permits the model to remove excessively large particles from the system by other than stirred settling means. Such a strategy seems reasonable for particles whose terminal settling velocity exceeds that of the mixing currents.

BRIEF DESCRIPTION OF SUBROUTINES

A flow chart of the main logic of QUICK is shown in the appended Figure 4 and each subroutine is briefly described.

To reduce the amount of computation, many of the coefficients in the aerosol equations are calculated at one time and stored in arrays for later use. Thus, the subroutines can be divided into two types, those involved in the initial setup of the problem (INPUT, DOUT, FACTORS, FILTER, INIT, KERN, LEAK, MESH, NSTOKE, OUT, RADIUS, REMOVE, SOURCE, SPLINE, AND XDP) and those used during problem solution (DEPO, DRIVE, EXTEND, OUTPUT, VARRGS). Subroutines SOURCE and KERN are recalled at the end of the aerosol source time and turbulent coagulation time, if appropriate.

The solution of the differential equations is performed by the GEAR differential equation solver package (DRIVE, INTERP, STIFF, COSET, PSET, DEC, and DOL). The GEAR package is treated as a "black box" by QUICK.

INPUT

All input to the QUICK code is performed by INPUT. All dimensioned input to the code is converted to the CGS measurement system. Temperature is converted to Kelvin.

INPUT is divided into four subgroups:

- Code control parameters which remain fixed for most problems.
- Dimensional input parameters which define the problem under consideration.
- Interpolation tables for variable source, gas-wall temperature difference, filter rate and efficiency, leak rate and trapping efficiency, source particle size and source particle standard deviation.
- Nondimensional parameters used for restarting a problem.

CUN

The Knudsen-Weber-Cunningham slip correction is applied by CUN. This routine is called by KERN and REMOVE.

DEPO

The cumulative mass removed by diffusion, thermophoresis, sedimentation, filtration, and leakage is determined by DEPO. The rate of mass loss for each size interval for each removal mechanism is calculated and the lost mass is determined by a simple Eulerian integration in order to optimize code running time. These values are used by OUTPUT.

DIFFUN

The rate of change of the number of particles in each size interval, required by the GEAR routine, is computed by subroutine DIFFUN. The first portion of the routine handles coagulation by two particle collisions. The second portion of the routine includes the effects of the source and removal terms.

DIFFUN uses the next to last and the last channel to accumulate the number and mass, respectively, of particles which grow beyond the range of particle size being considered. The number of channels in this range is NS-1. (See INIT and SOURCE for a discussion of the development of NS.) As the particle size distribution widens, NS is increased to include larger particles in the system of equations. (See EXTEND for a description of the channel extension procedure.)

DOUT

The nondimensional factors used for the QUICK calculations are printed by DOUT.

EXTEND

When coagulation necessitates the inclusion of an additional channel in the distribution, subroutine EXTEND performs the required operations. The GEAR routine is restarted with a reduced Δt, NS is incremented by 1.

The lost number and mass channel numbers are also incremented by 1 to maintain a running total for number and mass lost from the end of the distribution.

FACTORS

The QUICK code uses nondimensional factors in the internal calculations. These factors are calculated by FACTORS. Times are also nondimensionalized by division by the characteristic Brownian coagulation time $(K_o N_o)^{-1}$. The nondimensional factors computed here are printed by DOUT.

FILTER

FILTER determines the filter collection efficiency for particles of each size interval by linear interpolation of the filter efficiency table. LINTERP is used to perform the interpolation. If no efficiency table is available, FILTER assumes a collection efficiency of 1. A minimum of 4 points are required if an efficiency table is used. The removal rates are used by DEPO and DIFFUN to determine the filter effects.

INIT

Three initial distributions can be selected by the case input parameter. Two of these distributions are used when checking against special analytic solutions to the aerosol equation. The third distribution is the log normal distribution used for most aerosol work. INIT initializes the distribution for the selected case. In conjunction with the BMIN1 code control parameter, INIT determines NS which determines the number of channels which are considered by DIFFUN.

If the IRST code control parameter is 1, INIT will use an initial number distribution input by the user. This distribution must be in nondimensional form. The restart capability is used to restart after a central processor time limit, but can also be used to adapt QUICK to problems having two or more distinct source periods. All parts of multiple source problems must use the same total mass to use QUICK in this manner.

KERN

Several forms of the coagulation kernel are available in KERN. Two are for special analytic solution cases, while the third includes

Brownian and graviational coagulation and the fourth combines Brownian, gravitational and turbulent coagulation. If turbulent coagulation stops during the problem, KERN is recalled to recompute the kernel without turbulent coagulation.

LEAK

LEAK calculates the aerosol removal rates by a containment leak. Provision is made for particle size dependent trapping of particles within the cracks of the leak. A linear interpolation of the size dependent efficiency determines the fraction trapped and leaked. If no table of trapping efficiencies is provided LEAK assumes a trapping efficiency of zero. A minimum of 4 points are required for the trapping efficiency table. The trapping rates calculated here are used by DEPO to determine the mass trapped by the leak.

LINTERP

LINTERP is a general linear interpolation routine for arbitrary spacing of arguments. It is used to interpolate the input tables of data. It is used by FILTER, LEAK, VARRGS, VDTEMP, VFILTER, and VLEAK.

MESH

MESH determines the nodal spacing of the mass channels used by QUICK. The mass of each channel is taken to be the geometric mean of the left and right nodes of each channel except for the first channel where the arithmetic mean is used. For the general case, the spacing is equal on the logarithm of particle size.

NSTOKE

NSTOKE corrects for the non-Stokesian behavior of aerosol particles. An array VPLUS(I) is calculated which contains the ratio of the non-Stokesian over Stokesian settling velocity. SETTLE is used to determine the non-Stokesian settling velocity.

OUT

OUT calls DIFFUN to calculate the time derivative of each particle size channel and print it. This is useful in assessing the stiffness of a given problem, for example.

RADIUS

The mass equivalent radius and the natural log of the aerodynamic radius of the characteristic particle of each channel is calculated by RADIUS. These values are used by FILTER, LEAK and OUTPUT.

REMOVE

The removal rate coefficients for diffusional, gravitational and thermophoretic deposition are calculated in REMOVE. These coefficients are used in DEPO and DIFFUN.

SETTLE

SETTLE determines the non-Stokesian settling velocities used by NSTOKE. As discussed elsewhere in this report, empirical values of settling velocities for particle Reynold's numbers in excess of 1259 are not available. Above this Reynold's number, the correction at Re = 1259 is used.

SINTERP

SINTERP is a general cubic spline interpolation routine. Cubic spline coefficients calculated by SPLINE are used here to determine the ordinate or first two derivatives of an input table. SINTERP is called by VSOURCE to determine the slope of the cumulative mass curve when a time varying aerosol source is being used. Since SPLINE is used to process all of the input tables, SINTERP could be used in place of LINTERP discussed above; however, the step functions and slope discontinuities which can occur in several of these tables cause severe oscillations in the resulting spline functions in the region of the discontinuity. The cubic spline interpolation

is restricted to the cumulative source mass table because it does not contain these discontinuities.

SOURCE

SOURCE determines the value of the source coefficient used in the aerosol equation assuming a log normal source particle distribution. SOURCE determines the value of NS for cases which have no initial aerosol concentration. It is called by QUICK to evaluate the source coefficients at the start of the problem. It is called again at the source cutoff time to set all the source coefficients to zero. When the source possesses a time varying r_{gs} or σ_s, SOURCE is called by VARRGS to reevaluate the source coefficients before each step of the GEAR routine.

SPLINE

SPLINE is a general routine for calculation of the coefficients required for the SINTERP cubic spline interpolation routine. The end points are assumed to have second derivatives of one half the value of their adjacent points. The end point conditions are determined by QUICK using variables FØ and FN. SPLINE is used to process all the input data tables to maintain flexibility. All input data tables must be between 4 and 20 points to satisfy the requirements of SPLINE.

VARRGS

VARRGS handles the reevaluation of the source coefficients when a source with time varying r_{gs} or σ_s is specified. VARRGS uses LINTERP to determine the value of r_{gs} and/or σ_s at the midpoint of the current time step, then calls SOURCE to recalculate the source coefficients. If the change in the source distribution requires an increase in the channel number, VARRGS calls EXTEND.

VDTEMP

VDTEMP uses LINTERP to determine the gas-wall temperature difference. VDTEMP is called by DEPO and DIFFUN.

VFILTER

VFILTER uses LINTERP to calculate the filter volume fraction flow rate required by DEPO and DIFFUN.

VLEAK

VLEAK uses LINTERP to calculate the leak volume fraction flow rate required by DEPO and DIFFUN.

VSOURCE

VSOURCE uses SINTERP to calculate the slope of the cumulative mass curve required by DIFFUN.

XDP

XDP determines the channel number of the particle resulting from the collision of any two particles in the system. The mass of the resultant particles is apportioned between two channels so that mass is conserved in the system. The results of the calculations by XDP are used by the coagulation portion of DIFFUN.

OUTPUT

Output from QUICK is performed primarily by OUTPUT which is called after a user specified number of iterations of the GEAR package. The printout is divided into two sections. The first section shows the situation in the nondimensional form actually used in the QUICK calculations. In the second section, the dimensional parameters are given since these data are generally in the most useful form. The output from QUICK is discussed in more detail following the section on the input required for QUICK.

DESCRIPTION OF INPUT TO QUICK

A list of the input cards for QUICK is given in the next section. A detailed description of each input parameter is given below. Input to QUICK is formatted.

Card No.	Variable Name	Format	Description
1	TITLE	16A5	Up to 80 columns of title information can be included for printout at the start of the run.
2	CASE	A5	Controls the initial distribution calculated by INIT and the form of the coagulation collision kernel calculated by KERN. Six cases are currently recognized by QUICK: SCOTT, GOLVN, BROWN, GRAVE, BROGR and COMPL. SCOTT and GOLVN are used for cases which possess analytic solutions. BROWN uses a log normal initial distribution with Brownian coagulation only. GRAVE allows only gravitational coagulation. BROGR employs both Brownian and gravitational coagulation. These 5 cases consider coagulation only; no source or removal terms are included. The COMPL case employs all the resources of the QUICK code.
3	LSTEP	I10	QUICK calls the OUTPUT subroutine after every LSTEP iterations of the GEAR package. A value of 10 to 50 is recommended depending on the time resolution desired in the output.
4	NDIM	I10	Maximum size for the arrays used by XDP. The minimum value for NDIM can be calculated by setting NDIM = $N^2/2 + N$. The maximum value for NDIM is 5100.
5	DELR	E10.0	Smallest particle radius (micrometers) to be considered by QUICK.
6	RMAX	E10.0	Largest particle radius (micrometers) to be considered by QUICK. There is no maximum value for RMAX.
7	N	I10	Number of channels to be included between DELR and RMAX. QUICK will add channels as needed up to this number. The maximum value for N is 100; however, most problems work well with $40 < N < 60$. Computer running time is roughly proportional to N^2.

Card No.	Variable Name	Format	Description
8	DELT	E10.0	Initial time step (seconds) used by the GEAR package.
9	EPS	E10.0	Error criterion used by the GEAR routine when determining the step size. Small values of EPS yield the most accurate results but cause slower running due to small step size. Recommended values are $10^{-5} > EPS > 10^{-7}$.
10	MF	I10	Determines the solution technique used by the GEAR routine. Use MF = 22 for Gear's method.
11	BMIN1	E10.0	Determine the smallest number fraction which will be included at the start of the problem. BMIN1 should be chosen to encompass the peak of the mass distribution. A recommended value is BMIN1 = 1.0E-15.
12	BMIN2	E10.0	The fraction of the total suspended mass which can be lost before QUICK calls EXTEND. QUICK accumulates the mass lost from the end of the distribution in channel NS + 1. When the mass lost in this manner since the previous call to EXTEND exceeds BMIN2 times the total suspended mass, QUICK calls EXTEND to add a channel to the distribution.
13	IRST	I10	If IRST ≠ 0, QUICK requires cards 66 to 73 to perform a restart. The restart can also be used to produce an initial distribution which is not log normal.
14	RG	E10.0	The number geometric mean mass equivalent radius (micrometers) of the initial distribution. RG = R_{50} ($e^{-3 \ln^2 SIG}$). If RG is nonzero it is used with SIG to calculate the average particle mass XØ used for nondimensionalization.
15	SIG	E10.0	The logrithmic standard deviation of the initial particle size distribution. It is used with RG to calculate the average particle mass XØ used for nondimensionalization.
16	NØ	E10.0	The initial number concentration (particles/cm^3). If nonzero, it is used with XØ to calculate TMASS = XØ*NØ.

Card No.	Variable Name	Format	Description
17	T	E10.0	Initial time (seconds).
18	TMAX	E10.0	Final time (seconds).
19	TMASS	E10.0	Total initial aerosol mass (g/m^3). Used as g/cm^3 internally. If NØ = 0, TMASS is used with XØ to calculate $N\emptyset = \frac{TMASS}{X\emptyset}$. If NØ is non-zero, TMASS is recalculated as described for NØ; therefore, NØ and TMASS should not both be specified. TMASS is generally the easier parameter to determine.
20	ENERGY	E10.0	Turbulent energy dissipation rate density (cm^2/sec^3) in the aerosol system. Set equal to zero to ignore turbulent coagulation. QUICK makes no provision for time varying turbulence.
21	TENERGY	E10.0	Cut off time (seconds) for turbulent coagulation. TENERGY must be zero when ENERGY = 0.0.
22	PRES	E10.0	Characteristic gas pressure (atmospheres). QUICK makes no provision for time varying gas pressure.
23	TEMP	E10.0	Characteristic gas temperature (Celsius). QUICK makes no provision for time varying gas temperature.
24	DTEMP	E10.0	Gas-wall differential temperature (Celsius) used for thermophoretic deposition. If DTEMP > 0.0, Card 45 for NPT must be included.
25	RHOP	E10.0	Particle material density (g/cm^3).
26	CRATIO	E10.0	Ratio of gas to particle thermal conductivities used for calculation of thermophoretic deposition coefficients.
27	DELD	E10.0	Diffusion boundary layer thickness (cm).
28	DELTH	E10.0	Thermal boundary layer thickness (cm).
29	GEFF	E10.0	Gravitational coagulation collision efficiency. If 0.0 > GEFF > -9.9 $\varepsilon = 1.5(R2/(R1+R))^2$ is used. If GEFF < -10.0, the GEPS collision efficiency package[9] which is not included with QUICK is used to calculate the collision efficiency.

Card No.	Variable Name	Format	Description
30	SMR	E10.0	Source mass rate (g/m^3-sec). When both NØ and TMASS are zero, SMR and TS (below) are used to determine the total mass in the system: TMASS = SMR*TS. If SMR > 0.0 Card 42 for NPS must be included.
31	TS	E10.0	Source cutoff time (seconds).
32	RGS	E10.0	The number geometric mean mass equivalent radius (micrometers) of the source. RGS = RS_{50} ($e^{-3\ \ln^2 SIGS}$). If RG (Card 14), SIG (Card 15), NØ (Card 16) and TMASS (Card 19) are 0.0, the source parameters, SMR, TS, RGS and SIGS, are used to calculate the nondimensionalizing parameters NØ and XØ. If RGS > 0.0 Card 60 for NPR must be included. If a variable RGS is used (NPR, Card 60, > 0), the value for RGS should be near the maximum variable RGS value.
33	SIGS	E10.0	Logarithmic standard deviation of the source particle distribution. Used with RGS above to define the source distribution. If SIGS > 0.0 Card 13 for NPSIG must be included. If a variable SIGS is used (NPSIG, Card 63, > 0) the value for SIGS should be near the maximum variable SIGS value.
34	ASEDV	E10.0	Ratio of sedimentation area to total volume (cm^{-1}).
35	ADIFV	E10.0	Ratio of total internal surface area to total volume (cm^{-1}).
36	ATHV	E10.0	Ratio of total internal surface area for thermophoretic deposition to total volume (cm^{-1}). Generally ATHV = ADIFV except where a hot zone can form in the system with significantly greater thermophoretic deposition.
37	CHI	E10.0	Dynamic shape factor.
38	GAMMA	E10.0	Collision shape factor.
39	VF	E10.0	Volume fractional flow rate (sec^{-1}) for flow through a recirculating filter. If VF > 0.0 Card 48 for NPVF and Card 51 for NPF must be included.

Card No.	Variable Name	Format	Description
40	VL	E10.0	Volume fractional leak rate (sec^{-1}) for flow through a leak. If VL > 0.0 Card 54 for NPVL and Card 57 for NPL must be included.
41	VOL	E10.0	Total containment volume (m^3).

The following cards are to be included only when indicated by nonzero values on the indicated input cards.

Card No.	Variable	Format	Condition for Inclusion	Description
42	NPS	I10	SMR (Card 30) > 0.0	Number of points for time varying source. NPS can take any integer value from 0 to 20 except 1, 2, 3 and 4.
43	VSOURCE(NPS,1)	8E10.0	NPS (Card 42) > 0	Times (seconds) for cumulative source mass.(a)
44	VSOURCE(NPS,2)	8E10.0	NPS (Card 42) > 0	Cumulative source mass (g/m^3).(a)
45	NPT	I10	DTEMP (Card 24) > 0.0	Number of points for time varying temperature difference. NPT can take any integer value from 0 to 20 except 1, 2 and 3.
46	VDTEMP(NPT,1)	8E10.0	NPT (Card 45) > 0	Times (seconds) for temperature difference.(a)
47	VDTEMP (NPT,2)	8E10.0	NPT (Card 45) > 0	Gas-wall temperature difference (Celsius).(a)
48	NPVF	I10	VF (Card 39) > 0.0	Number of points for variable filter rate. See NPT (Card 45) for allowed values.
49	VFIL(NPVF,1)	8E10.0	NPVF (Card 48) > 0	Times (seconds) for variable filter rate.(a)
50	VFIL(NPVF,2)	8E10.0	NPVF (Card 48) > 0	Volume fractional filter flow rate (sec^{-1}).(a)
51	NPF	I10	VF (Card 39) > 0.0	Number of points for variable filter collection efficiency. See NPT (Card 45) for allowed values. If NPF = 0 a constant filter efficiency of 1.0 is assumed.

Card No.	Variable	Format	Condition for Inclusion	Description
52	EPSF(NPF,1)	8E10.0	NPF (Card 51) > 0	Particle radii (micrometers) for variable filter efficiency.[a]
53	EPSF(NPF,2)	8E10.0	NPF (Card 51) > 0	Filter collection efficiencies. Allowed values range from 0.0 for no collection to 1.0 for 100% collection.[a]
54	NPVL	I10	VL (Card 40) > 0.0	Number of points for variable leak rate. See NPT (Card 45) for allowed values.
55	VLK(NPVL,1)	8E10.0	NPVL (Card 54) > 0	Times (seconds) for variable leak rate.[a]
56	VLK(NPVL,2)	8E10.0	NPVL (Card 54) > 0	Volume fractional leak flow rates (sec^{-1}).[a]
57	NPL	I10	VL (Card 40) > 0.0	Number of points for variable leak trapping efficiency. See NPT (Card 45) for allowed values. If NPL = 0 a constant leak trapping efficiency of 0.0 is assumed.
58	EPSL(NPL,1)	8E10.0	NPL (Card 57) > 0	Particle radii (micrometers) for variable leak trapping efficiency.[a]
59	EPSL(NPL,2)	8E10.0	NPL (Card 57) > 0	Leak trapping efficiency. Allowed values range from 0.0 for no trapping to 1.0 for 100% trapping.[a]
60	NPR	I10	RGS (Card 32) > 0.0	Number of points for variable RGS. See NPT (Card 45) for allowed values.
61	VRGS(NPR,1)	8E10.0	NPR (Card 60) > 0	Times (seconds) for variable RGS.[a]
62	VRGS(NPR,2)	8E10.0	NPR (Card 60) > 0	RGS values.[a]
63	NPSIG	I10	SIGS (Card 33) > 0.0	Number of points for variable SIGS. See NPT (Card 45) for allowed values.
64	VSIGS(NPSIG,1)	8E10.0	NPSIG (Card 63) > 0	Times (seconds) for variable SIGS.[a]

Card No.	Variable	Format	Condition for Inclusion	Description
65	VSIGS(NPSIS,2)	8E10.0	NPSIG (Card 63) > 0	SIGS values.(a)
66	L	I10	IRST (Card 13) > 0	Starting iteration number.
67	DIFMAS	E10.0	IRST (Card 13) > 0	Nondimensional diffusion mass deposited.
68	THMAS	E10.0	IRST (Card 13) > 0	Nondimensional thermophoretic mass deposited.
69	SEDMAS	E10.0	IRST (Card 13) > 0	Nondimensional sedimented mass deposited.
70	FILMAS	E10.0	IRST (Card 13) > 0	Nondimensional mass filtered.
71	TRAPMAS	E10.0	IRST (Card 13) > 0	Nondimensional mass trapped.
72	LEAKMAS	E10.0	IRST (Card 13) > 0	Nondimensional mass leaked.
73	B(N+1)	E10.0	IRST (Card 13) > 0	Nondimensional number histogram values for every channel followed by the last mass histogram value and enough zero entries to exceed N+1.(a)

(a) Eight entries can be placed on one card. Use additional cards if more than eight entries are required.

LIST OF INPUT CARDS

Variable	Format	Condition	Description
1 TITLE	16A5	Required	Problem title.
2 CASE	A5	Required	QUICK operation mode (COMPL)
3 LSTEP	I10	Required	Output interval.
4 NDIM	I10	Required	Maximum dimension used by XDP.
5 DELR	E10.0	Required	Minimum radius (micrometers).
6 RMAX	E10.0	Required	Maximum radius (micrometers).
7 N	I10	Required	Number of channels.
8 DELT	E10.0	Required	Initial time step (seconds).
9 EPS	E10.0	Required	Gear routine error criterion.
10 MF	I10	Required	MF = 22.
11 BMIN1	E10.0	Required	Initial channel cutoff.
12 BMIN2	E10.0	Required	Channel extension criterion.
13 IRST	I10	Required	Restart if IRST >0.
14 RG	E10.0	Required	Initial number geometric mean mass equivalent radius (micrometers).
15 SIG	E10.0	Required	Initial distribution logarithmic standard deviation.
16 NØ	E10.0	Required	Initial number concentration (particles/cm^3).
17 T	E10.0	Required	Initial time (seconds).
18 TMAX	E10.0	Required	Final time (seconds).
19 TMASS	E10.0	Required	Initial aerosol mass (g/m^3).
20 ENERGY	E10.0	Required	Turbulent energy (cm^2/sec^3).
21 TENERGY	E10.0	Required	Turbulent coagulation cufoff time (seconds).
22 PRES	E10.0	Required	Pressure (atmospheres).
23 TEMP	E10.0	Required	Temperature (Celsius).
24 DTEMP	E10.0	Required	Gas-wall temperature difference (Celsius).
25 RHOP	E10.0	Required	Particle density (g/cm^3).
26 CRATIO	E10.0	Required	Ratio gas to particle thermal conductivities.
27 DELD	E10.0	Required	Diffusion boundary layer thickness (cm).
28 DELTH	E10.0	Required	Thermophoretic deposition boundary layer thickness (cm).
29 GEFF	E10.0	Required	Graviational coagulation collision efficiency.
30 SMR	E10.0	Required	Source mass rate (g/m^3 sec).

Variable	Format	Condition	Description
31 TS	E10.0	Required	Source cut off time (seconds).
32 RGS	E10.0	Required	Source number geometric mean mass equivalent radius (micrometers).
33 SIGS	E10.0	Required	Source distribution logarithmic standard deviation.
34 ASEDV	E10.0	Required	Sedimentation area/volume (cm^{-1}).
35 ADIFV	E10.0	Required	Total area/volume (cm^{-1}).
36 ATHV	E10.0	Required	Thermophoretic deposition area/volume (cm^{-1}).
37 CHI	E10.0	Required	Dynamic shape factor.
38 GAMMA	E10.0	Required	Collision shape factor.
39 VF	E10.0	Required	Volume fraction filtered (sec^{-1}).
40 VL	E10.0	Required	Volume fraction leaked (sec^{-1}).
41 VOL	E10.0	Required	Total volume.
42 NPS	I10	SMR > 0.0	Number of points for variable source.
43 VSOURCE(NPS,1)	8E10.0	NPS > 0	Variable source times (seconds).
44 VSOURCE(NPS,2)	8E10.0	NPS > 0	Cumulative source mass (g/m^3).
45 NPT	I10	DTEMP > 0.0	Number of points for variable temperature difference.
46 VDTEMP(NPT,1)	8E10.0	NPT > 0	Variable temperature difference times (seconds).
47 VDTEMP(NPT,2)	8E10.0	NPT > 0	Gas-wall temperature differences (Celsius).
48 NPVF	I10	VF > 0.0	Number of points for variable filter rate.
49 VFIL(NPVF,1)	8E10.0	NPVF > 0	Variable filter rate times (seconds).
50 VFIL(NPVF,2)	8E10.0	NPVF > 0	Volume fractional filter flow rates (sec^{-1}).
51 NPF	I10	VF > 0.0	Number of points for filter collection efficiency. If NPF = 0, a constant collection efficiency of 1.0 is assumed.
52 EPSF(NPF,1)	8E10.0	NPF > 0	Particle radii (micrometers) for filter collection efficiency.
53 EPSF(NPF,2)	8E10.0	NPF > 0	Filter collection efficiency.
54 NPVL	I10	VL > 0.0	Number of points for variable leak rate.
55 VLK(NPVL,1)	8E10.0	NPVL > 0	Variable leak rate times (seconds).
56 VLK(NPVL,2)	810.0	NPVL > 0	Volume fractional leak flow rate (sec^{-1}).
57 NPL	I10	VL > 0.0	Number of points for variable leak trapping efficiency. If NPL = 0, a constant trapping efficiency of 0.0 is assumed.
58 EPSL(NPL,1)	8E10.0	NPL > 0	Particle radii (micrometers) for leak trapping efficiency.

Variable	Format	Condition	Description
59 EPSL(NPL,2)	8E10.0	NPL > 0	Leak trapping efficiency.
60 NPR	I10	RGS > 0.0	Number of points for variable RGS.
61 VRGS(NPR,1)	8E10.0	NPR > 0	Times (seconds) for variable RGS.
62 VRGS(NPR,2)	8E10.0	NPR > 0	RGS values (micrometers).
63 NPSIG	I10	SIGS > 0.0	Number of points for variable SIGS.
64 VSIGS(NPSIG,1)	8E10.0	NPSIG > 0	Times (seconds) for variable SIGS.
65 VSIGS(NPSIG,2)	8E10.0	NPSIG > 0	SIGS values.
66 L	I10	IRST > 0	Restart beginning iteration number.
67 DIFMAS	E10.0	IRST > 0	Nondimensional mass deposited by diffusion.
68 THMAS	E10.0	IRST > 0	Nondimensional mass deposited by thermophoresis.
69 SEDMAS	E10.0	IRST > 0	Nondimensional mass deposited by sedimentation.
70 FILMAS	E10.0	IRST > 0	Nondimensional mass filtered.
71 TRAPMAS	E10.0	IRST > 0	Nondimensional mass trapped by leak.
72 LEAKMAS	E10.0	IRST > 0	Nondimensional mass leaked from containment.
73 B(N+1)	8E10.0	IRST > 0	Nondimensional number histogram values and lost mass bin with enough zeroes to exceed N+1 entries.

CODE OUTPUT

The output produced by the QUICK code can be divided into four sections:

- The input parameters printed by INPUT
- The nondimensional factors and normalizing parameters calculated by FACTORS and printed by DOUT.
- The time derivatives of the nondimensional number histogram calculated by DIFFUN and printed by OUT.
- The aerosol conditions printed by OUTPUT after a selected number of iterations.

The significance of the input parameters is discussed in the section on INPUT to QUICK. For a discussion of the nondimensional factors, see the description of the QUICK model. The printout from OUT comprises four columns showing the channel number, nondimensional mass of the characteristic particle, the nodal spacing on the mass axis and the time derivatives of the nondimensional number histogram at the start of the problem.

The output from the QUICK code OUTPUT routine is described below (see the sample problem output). It can be conveniently divided into two parts: a nondimensional section used in the QUICK calculations and a dimensional section in which the QUICK results are expressed in commonly used units. The numbers shown in the nondimensional number histogram column are the values actually used in the aerosol equations, all other results are derived from the nondimensional number histogram.

The first value in the nondimensional section is the iteration number followed by the most recent time step used by GEAR, DELT. The mass lost by each of the deposition mechanisms and the total mass removed, all calculated by DEPO, is printed next. The next line shows the nondimensional time, number normalized against NØ and suspended mass normalized against TMASS. The last portion of the nondimensional section displays the particle size distribution in several ways. The Index column is the channel number. The X column is the nondimensional characteristic mass for each channel.

The number distribution density is printed in column three and the mass distribution density is printed in column four. The number histogram is printed in column five. The mass histogram is printed in column six. The last column gives $\partial(\tilde{n}(\tilde{x},t)\tilde{x})/\partial\ln\tilde{x}$.

The last entries in the number and mass histogram columns are the values in the number and mass bins. QUICK maintains these bins to keep track of particles which grow beyond the current maximum size. The amount of mass permitted to be lost is controlled by input parameter BMIN2. The sum of the total mass removed, the suspended mass and the mass in this bin will be 1.0 with allowances for errors caused by the discretization and the inaccuracy of the simple Eulerian intergration scheme used by DEPO.

The dimensional portion of the output shows the time expressed as seconds, minutes and hours, followed by several characteristic radii of the distribution and the standard deviation of the particle distribution. The total number of particles and amount of mass suspended are also shown. The mass of aerosol removed by each of the deposition mechanisms is printed next. The last part of the dimensional output shows the particle distribution in dimensional form. The REQU column shows the mass equivalent radius for the characteristic particle of each channel. The RAERO column shows the corresponding aerodynamic radius. The number and mass columns give the number and mass present in each channel. The last column gives $\partial(n(x,t)x)/\partial\ln r$.

Restarting QUICK

The values used for restarting QUICK are all taken from the non-dimensional section. The iteration number, L, and the fraction of mass removed by each of the deposition mechanisms is shown. The values of B(I) from 1 to NS are contained in the number histogram column. The last entry in this column represents the cumulative number of particles which have become too large to be represented in the distribution. Since only the largest particles are lost in this way, the number of particles shown here is very small. As additional channels are added through the extension process, this number bin is moved to higher channel numbers.

The fraction of mass lost from the distribution is shown in the last entry in the mass histogram column. This value is handled as the NS+1 channel in QUICK. During a restart, INIT searches backward through the B(I)'s read in, for the first nonzero B(I) value, which is assigned to the mass bin channel. The value of NS is set equal to the mass bin channel minus 1. If all N channels were not used before a restart, enough 0.0 values must be included after the mass bin value so that QUICK finds N+1 entries for B(I).

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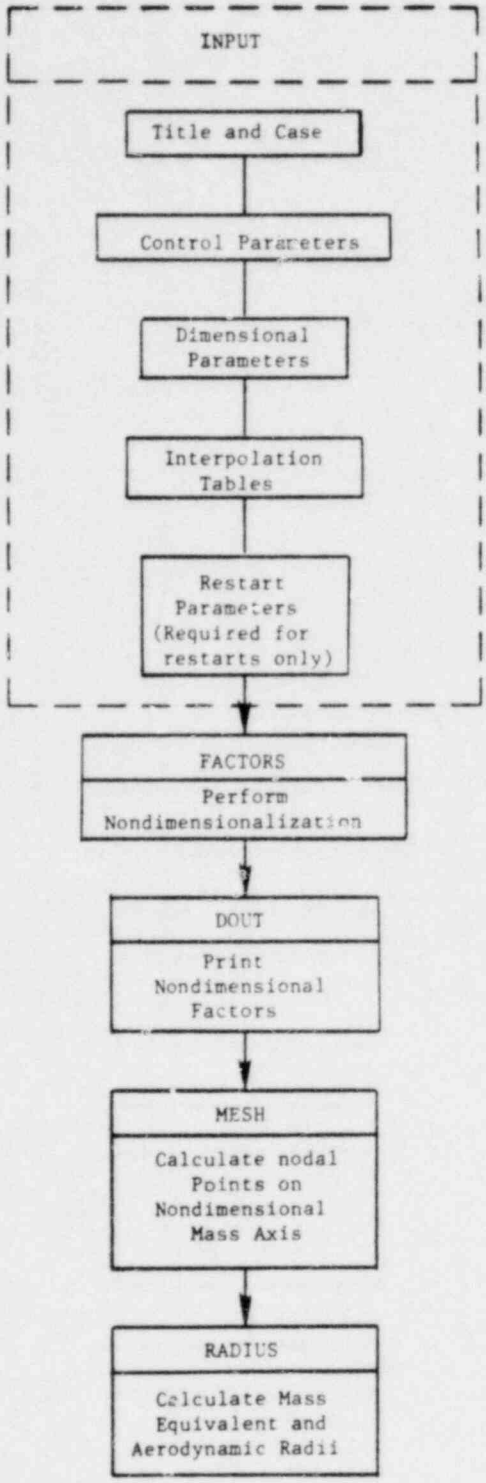
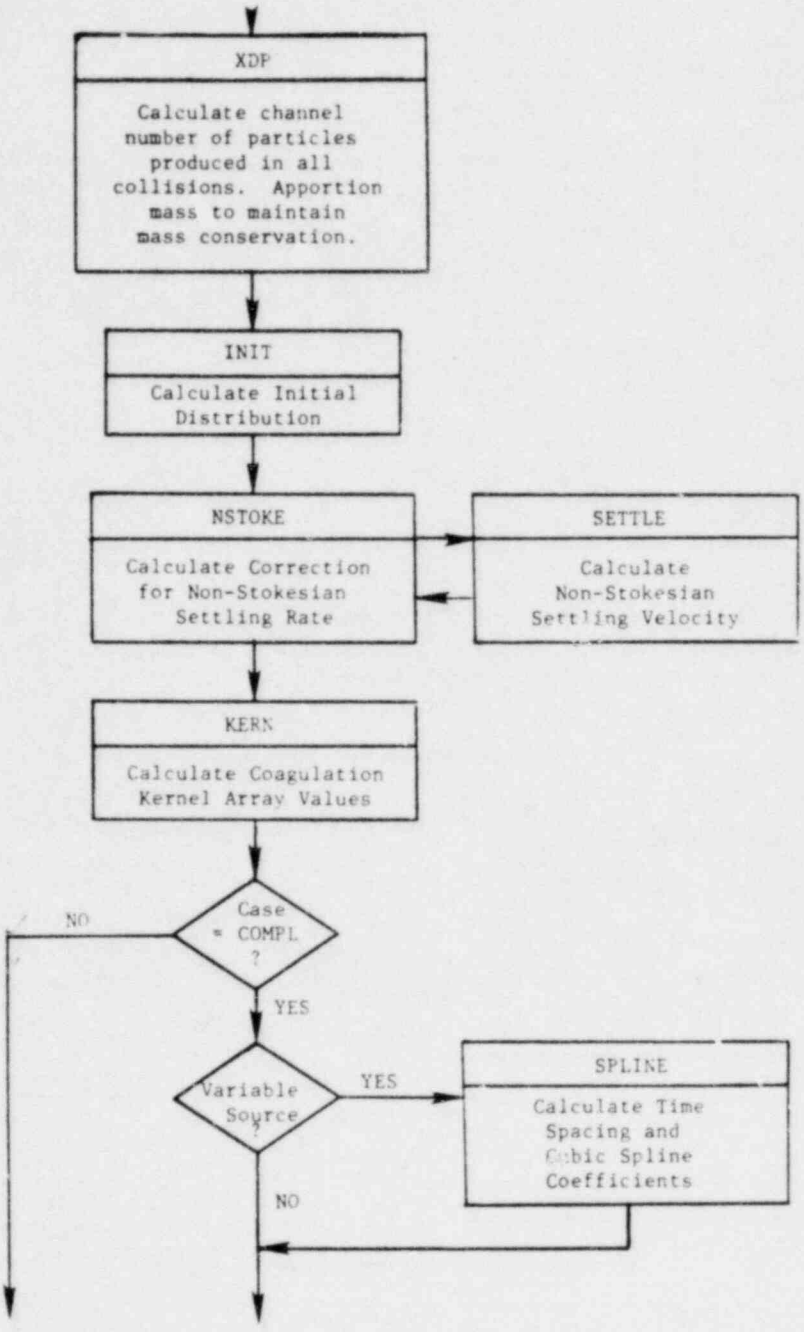
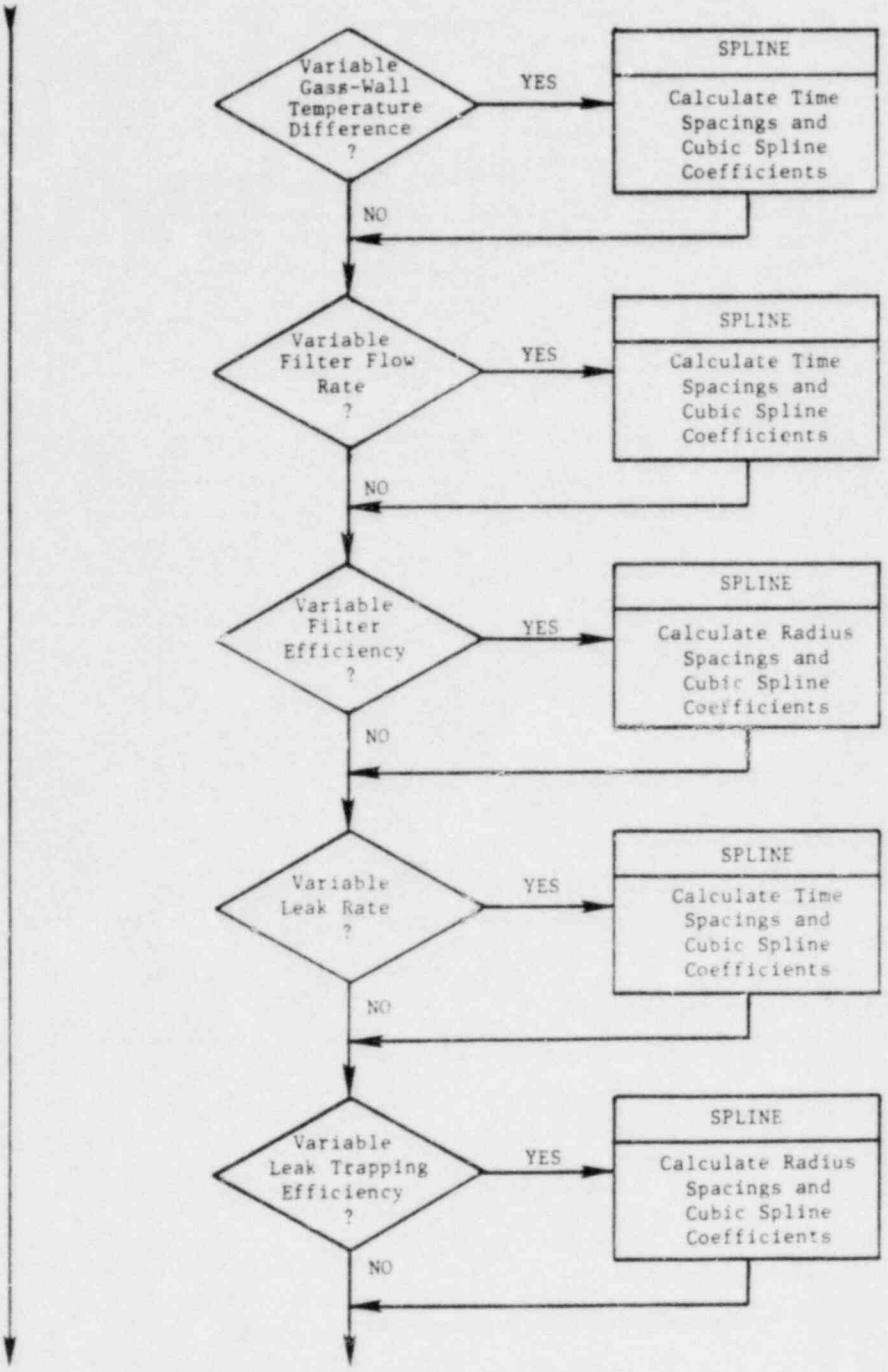
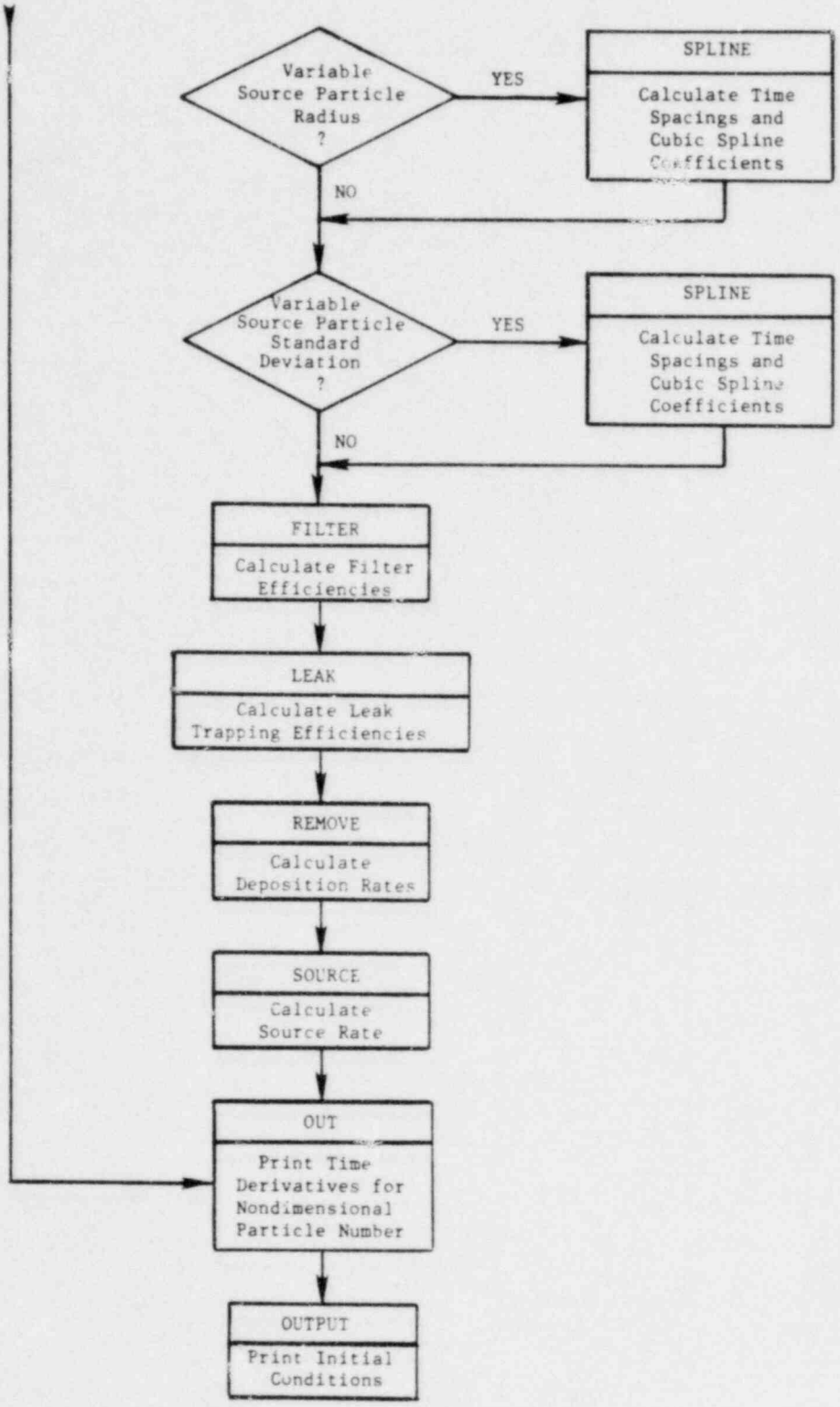
**Available for purchase from the National Technical Information Service.

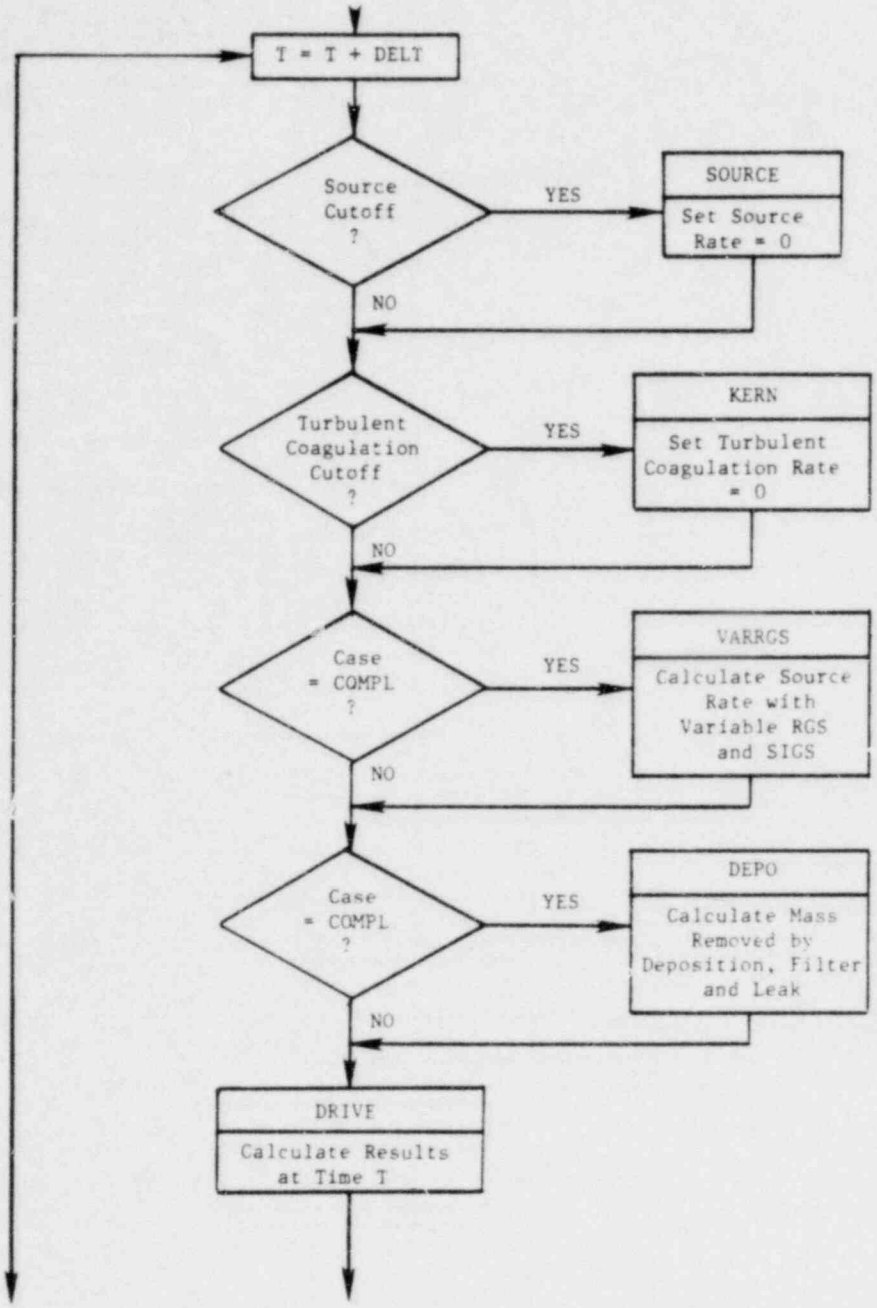
FLOW CHART OF THE QUICK CODE

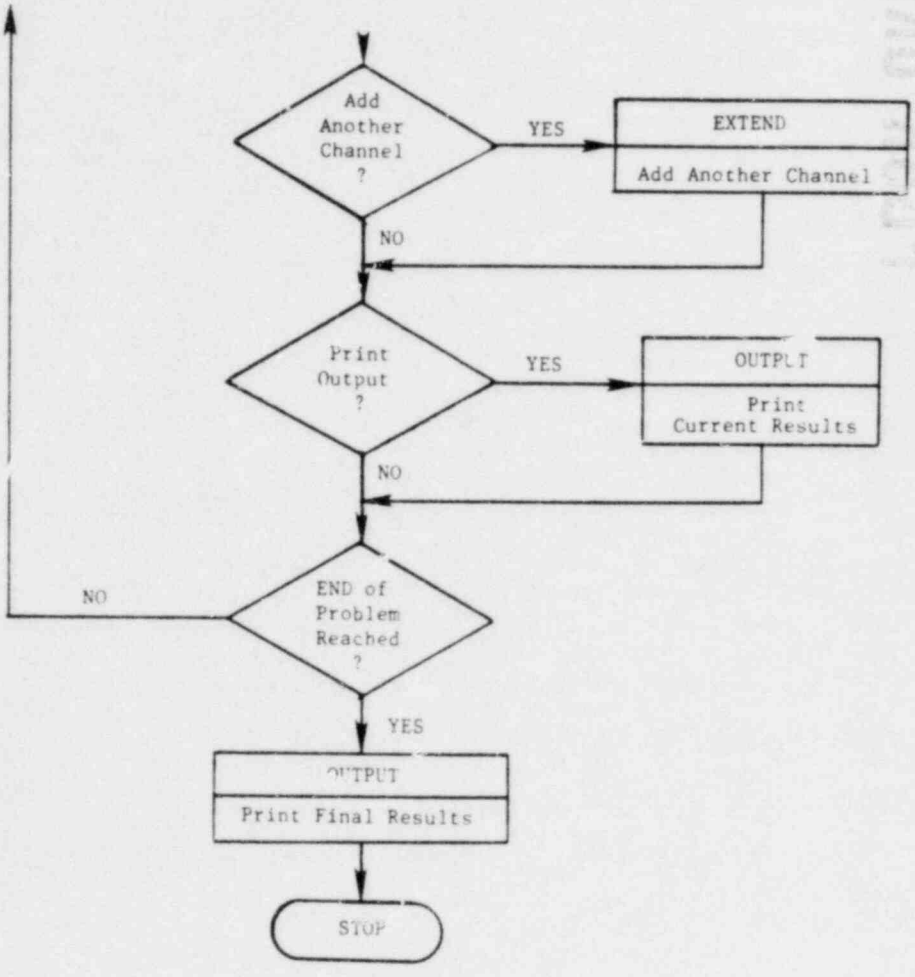





Variable Gass-Wall Temperature Difference ?
YES
SPLINE
Calculate Time Spacings and Cubic Spline Coefficients
NO
Variable Filter Flow Rate ?
YES
SPLINE
Calculate Time Spacings and Cubic Spline Coefficients
NO
Variable Filter Efficiency ?
YES
SPLINE
Calculate Radius Spacings and Cubic Spline Coefficients
NO
Variable Leak Rate ?
YES
SPLINE
Calculate Time Spacings and Cubic Spline Coefficients
NO
Variable Leak Trapping Efficiency ?
YES
SPLINE
Calculate Radius Spacings and Cubic Spline Coefficients
NO




T = T + DELT
Source Cutoff ?
YES
SOURCE
Set Source Rate = 0
NO
Turbulent Coagulation Cutoff ?
YES
KERN
Set Turbulent Coagulation Rate = 0
NO
Case = COMPL ?
YES
VARRGS
Calculate Source Rate with Variable RGS and SIGS
NO
Case = COMPL ?
YES
DEPO
Calculate Mass Removed by Deposition, Filter and Leak
NO
DRIVE
Calculate Results at Time T



QUICK USER MANUAL EXAMPLE PROBLEM 84-01-R1

DIMENSIONAL QUICK AEROSOL BEHAVIOR CODE
03-05-81 VERSION

COMPL CASE

** CODE CONTROL PARAMETERS **

LSTEP	20	
NDIM	1500	
DELR	.10000000E-01	MICROMETERS
RMAX	.10000000E+03	MICROMETERS
N	53	
DELT	.10000000E-02	
EPS	.10000000E-04	
MF	22	
PMIN1	.10000000E-14	
PMIN2	.10000000E-03	
IRST	0	RESTART PARAMETER

** DIMENSIONAL INPUT PARAMETERS **

RG	.30000000E+00	MICROMETERS
SIG	.20000000E+01	
N0	0.	PARTICLES/CM**3
T	0.	SEC
TMAX	.10000000E+03	SEC
TMASS	.20000000E+02	G/M**3
ENERGY	.10000000E+04	LM**2/SEC**3
TENERGY	.10000000E+02	SEC
PRES	.10000000E+01	ATMOSPHERES
TEMP	.50000000E+02	CELSIUS
DTEMP	.20000000E+02	CELSIUS
RHOP	.27000000E+01	G/CM**3
CRATIO	.10000000E+01	
DELD	.10000000E-01	CM
DELTH	.10000000E+01	CM
GEFF	-.10000000E+01	
SMR	.25000000E+01	G/(M**3*SEC)
TS	.90000000E+01	SEC
RGS	.70000000E+00	MICROMETERS
SIGS	.30000000E+01	
ASEDV	.10000000E-01	1/CM
ACIFV	.10000000E+00	1/CM
ATHV	.10000000E+00	1/CM
CHI	.13000000E+01	
GAMMA	.50000000E+01	
VF	.10000000E-05	VOLUME FRACTION FILTERED/SEC
VL	.11570000E-06	VOLUME FRACTION LEAKED/SEC
VOL	.10000000E+03	CONTAINMENT VOLUME (M**3)

NPS 7 POINTS FOR TIME VARYING SOURCE

TIME(SEC)	0.	.10000E+01	.20000E+01	.40000E+01	.60000E+01	.70000E+01	.80000E+01
CUMULATIVE SOURCE MASS(G/M**3)	0.	.65000E+01	.11000E+02	.16500E+02	.19000E+02	.19500E+02	.20000E+02

NPT 5 POINTS FOR TIME VARYING TEMPERATURE DIFFERENCE

TIME(SEC)	0.	.30000E+01	.80000E+01	.10000E+02	.50000E+02
TEMPERATURE DIFFERENCE(C)	0.	.10000E+02	.20000E+02	.15000E+02	.50000E+01

NPVF 5 POINTS FOR VARIABLE FILTER RATE

TIME(SEC)	.20000E+01	.50000E+01	.80000E+01	.30000E+02	.70000E+02
FRACTIONAL FLOW RATE/SEC	0.	.10000E-05	.10000E-04	.70000E-04	.20000E-05

NPF 14 POINTS FOR FILTER EFFICIENCY

RADIUS(MICROMETERS)	0.	.10000E-01	.20000E-01	.33000E-01	.50000E-01	.10000E+00	.20000E+00
.30000E+00	.50000E+00	.10000E+01	.20000E+01	.30000E+01	.50000E+01	.10000E+02	
EFFICIENCY	.10000E+01	.10000E+01	.95000E+00	.70000E+00	.45000E+00	.25000E+00	.20000E+00
.18000E+00	.22000E+00	.40000E+00	.60000E+00	.90000E+00	.99000E+00	.10000E+01	

NPVL 0 POINTS FOR VARIABLE LEAK RATE

NPL 14 POINTS FOR LEAK TRAPPING EFFICIENCY

RADIUS(MICROMETERS) 0. .10000E-01 .20000E-01 .33000E-01 .50000E-01 .10000E+00 .20000E+00
.30000E+00 .50000E+00 .10000E+01 .20000E+01 .30000E+01 .50000E+01 .10000E+02

EFFICIENCY .10000E+01 .10000E+01 .95000E+00 .70000E+00 .45000E+00 .25000E+00 .20000E+00
.18000E+00 .22000E+00 .40000E+00 .60000E+00 .90000E+00 .99000E+00 .10000E+01

NPF 5 POINTS FOR TIME VARYING RGS

TIME(SEC) 0. .20000E+01 .40000E+01 .60000E+01 .80000E+01

RGS .30000E+00 .50000E+00 .10000E+01 .60000E+00 .50000E+00

NPSIG 5 POINTS FOR TIME VARYING SIGS

TIME(SEC) 0. .20000E+01 .40000E+01 .60000E+01 .80000E+01

SIGS .17000E+01 .20000E+01 .25000E+01 .30000E+01 .25000E+01

** NONDIMENSIONAL FACTORS **

SRGC	SOURCE FACTOR	.85192719E-01	
GDPC	GRAVITATIONAL DEPOSITION FACTOR	.19973416E-01	
DFGD	DIFFUSIONAL DEPOSITION FACTOR	.17139833E-01	
THGD	THERMOPHORETIC DEPOSITION FACTOR	.73559321E+02	
GCBC	GRAVITATIONAL COAGULATION FACTOR	.44979227E+01	
TCF 1	TURBULENT COAGULATION FACTOR	.12475010E+01	GRADIENT
TCF2	TURBULENT COAGULATION FACTOR	.45375233E+00	INERTIA
VFGD	FILTER FLOW RATE FACTOR	.11396717E-01	
VLGD	LEAK FLOW RATE FACTOR	.13146002E-02	
KN	KNUDSEN NUMBER	.21199314E-01	
RG	RELATIVE MEDIAN INITIAL RADIUS	.48642156E+00	
RGS	RELATIVE MEDIAN SOURCE RADIUS	.11349836E+01	

NONDIMENSIONALIZED TIMES

TMAX		.43930674E+00
TENERGY	TURBULENT COAGULATION CUT-OFF	.43930674E-01
TS	SOURCE CUTOFF	.35144539E-01

DIMENSIONAL NORMALIZING PARAMETERS

AVERAGE PARTICLE MASS(X0)	.26532462E-11	GRAMS
K0	.58273447E-09	CM**3/SEC
INITIAL PARTICLE NUMBER (N0)	.75373359E+07	PARTICLES/CM**3
CHARACTERISTIC TIME (1/K0*N0)	.22763138E+03	SEC

** DIMENSION OF XOP IS 1431 **

INDEX	X	DX	BDOT
1	.213E-05	.426E-05	-.603E-04
2	.562E-05	.314E-05	-.116E-03
3	.977E-05	.547E-05	-.311E-03
4	.170E-04	.950E-05	-.783E-03
5	.295E-04	.165E-04	-.186E-02
6	.512E-04	.287E-04	-.420E-02
7	.891E-04	.498E-04	-.962E-02
8	.155E-03	.866E-04	-.184E-01
9	.269E-03	.151E-03	-.358E-01
10	.467E-03	.262E-03	-.663E-01
11	.812E-03	.455E-03	-.117E+00
12	.141E-02	.790E-03	-.196E+00
13	.245E-02	.137E-02	-.313E+00
14	.426E-02	.239E-02	-.474E+00
15	.741E-02	.415E-02	-.681E+00
16	.129E-01	.720E-02	-.927E+00
17	.224E-01	.125E-01	-.119E+01
18	.389E-01	.218E-01	-.145E+01
19	.676E-01	.378E-01	-.167E+01
20	.117E+00	.657E-01	-.181E+01
21	.204E+00	.114E+00	-.188E+01
22	.355E+00	.198E+00	-.173E+01
23	.616E+00	.345E+00	-.150E+01
24	.107E+01	.599E+00	-.116E+01
25	.186E+01	.104E+01	-.792E+00
26	.323E+01	.181E+01	-.453E+00
27	.562E+01	.314E+01	-.198E+00
28	.977E+01	.547E+01	-.426E-01
29	.170E+02	.950E+01	.277E-01
30	.295E+02	.165E+02	.447E-01
31	.512E+02	.287E+02	.376E-01
32	.891E+02	.498E+02	.252E-01
33	.155E+03	.866E+02	.150E-01
34	.269E+03	.151E+03	.860E-02
35	.467E+03	.262E+03	.513E-02
36	.812E+03	.455E+03	.320E-02
37	.141E+04	.790E+03	.208E-02
38	.245E+04	.137E+04	.138E-02
39	.426E+04	.239E+04	.913E-03
40	.741E+04	.415E+04	.595E-03
41	.129E+05	.720E+04	.378E-03
42	.224E+05	.125E+05	.235E-03
43	.389E+05	.218E+05	.142E-03
44	.676E+05	.378E+05	.833E-04
45	.117E+06	.657E+05	.476E-04
46	.204E+06	.114E+06	.264E-04
47	.355E+06	.198E+06	.143E-04
48	.616E+06	.345E+06	.748E-05
49	.107E+07	.599E+06	.382E-05
50	.186E+07	.104E+07	.189E-05
51	.323E+07	.181E+07	.913E-06
52	.562E+07	.314E+07	.428E-06
53	.977E+07	.547E+07	0.

ITERATION NUMBER 20

DELT .55569304E-0[illegible]

MASS REMOVED BY DIFFUSION= .171E-08
MASS REMOVED BY THERMOPHORSIS= .566E-05
MASS REMOVED BY SEDIMENTATION= .169E-03
MASS REMOVED BY FILTER= 0.
MASS TRAPPED BY LEAK= .101E-07
MASS LEAKED FROM CONTAINMENT= .103E-07
TOTAL MASS REMOVED= .175E-03

TIME= .744E-03 NUMBER= .113E+01 MASS= .107E+01

INDEX	X	NUM. DIS.	MASS DIS.	NUM. MIS.	MASS MIS.	NUM. DIS.*X**2
1	.213E-05	.[illegible]51E-01	.181E-06	.353E-06	.773E-12	.387E-12
2	.562E-05	.353E+00	.198E-05	.111E-05	.624E-11	.111E-10
3	.977E-05	.712E+00	.695E-05	.[illegible]39E-05	.380E-10	.679E-10
4	.170E-04	.133E+01	.226E-04	.[illegible]26E-04	.214E-09	.383E-09
5	.295E-04	.231E+01	.660E-04	.380E-04	.112E-08	.200E-08
6	.512E-04	.371E+01	.190E-03	.107E-03	.546E-08	.976E-08
7	.891E-04	.567E+01	.496E-03	.279E-03	.247E-07	.442E-07
8	.155E-03	.778E+01	.120E-02	.674E-03	.104E-06	.186E-06
9	.269E-03	.101E+02	.272E-02	.152E-02	.410E-06	.732E-06
10	.467E-03	.123E+02	.574E-02	.321E-02	.150E-05	.268E-05
11	.812E-03	.139E+02	.113E-01	.633E-02	.514E-05	.918E-05
12	.141E-02	.147E+02	.208E-01	.116E-01	.164E-04	.296E-04
13	.245E-02	.146E+02	.358E-01	.200E-01	.491E-04	.877E-04
14	.426E-02	.135E+02	.575E-01	.322E-01	.137E-03	.245E-03
15	.741E-02	.116E+02	.862E-01	.493E-01	.358E-03	.639E-03
16	.129E-01	.937E+01	.121E+00	.675E-01	.869E-03	.155E-02
17	.224E-01	.702E+01	.157E+00	.873E-01	.197E-02	.352E-02
18	.[illegible]E-01	.[illegible]89E+01	.190E+00	.105E+00	.414E-02	.739E-02
19	.676E-01	.316E+01	.213E+00	.113E+00	.807E-02	.144E-01
20	.117E+00	.189E+01	.222E+00	.124E+00	.146E-01	.260E-01
21	.204E+00	.104E+01	.213E+00	.113E+00	.243E-01	.435E-01
22	.355E+00	.535E+00	.190E+00	.106E+00	.376E-01	.673E-01
23	.616E+00	.254E+00	.156E+00	.875E-01	.539E-01	.964E-01
24	.107E+01	.112E+00	.120E+00	.670E-01	.718E-01	.128E+00
25	.186E+01	.458E-01	.853E-01	.477E-01	.888E-01	.159E+00

26	.323E+01	.175E-01	.567E-01	.317E-01	.103E+00	.183E+00
27	.562E+01	.526E-02	.352E-01	.137E-01	.111E+00	.138E+00
28	.977E+01	.209E-02	.204E-01	.114E-01	.112E+00	.199E+00
29	.170E+02	.653E-03	.111E-01	.620E-02	.105E+00	.188E+00
30	.295E+02	.191E-03	.563E-02	.355E-02	.929E-01	.166E+00
31	.512E+02	.521E-04	.267E-02	.160E-02	.766E-01	.137E+00
32	.891E+02	.133E-04	.118E-02	.663E-03	.590E-01	.105E+00
33	.155E+03	.316E-05	.489E-03	.276E-03	.424E-01	.757E-01
34	.269E+03	.700E-06	.188E-03	.105E-03	.284E-01	.507E-01
35	.467E+03	.145E-06	.676E-04	.378E-04	.177E-01	.316E-01
36	.812E+03	.278E-07	.226E-04	.126E-04	.103E-01	.183E-01
37	.141E+04	.497E-08	.702E-05	.393E-05	.554E-02	.931E-02
38	.245E+04	.829E-09	.203E-05	.114E-05	.279E-02	.499E-02
39	.426E+04	.129E-09	.549E-06	.307E-06	.131E-02	.234E-02
40	.741E+04	.186E-10	.138E-06	.772E-07	.572E-03	.102E-02
41	.129E+05	.251E-11	.323E-07	.181E-07	.232E-03	.415E-03
42	.224E+05	.314E-12	.703E-08	.394E-08	.880E-04	.157E-03
43	.389E+05	.367E-13	.143E-08	.733E-09	.310E-04	.555E-04
44	.676E+05	.399E-14	.269E-09	.151E-09	.102E-04	.182E-04
45	.117E+06	.403E-15	.474E-10	.255E-10	.311E-05	.556E-05
46	.204E+06	.388E-16	.775E-11	.434E-11	.885E-06	.158E-05
47	.355E+06	.333E-17	.118E-11	.660E-12	.234E-05	.418E-06
48	.616E+06	.271E-18	.167E-12	.934E-13	.575E-07	.103E-06
49	.107E+07	.205E-19	.220E-13	.123E-13	.132E-07	.235E-07
50	.186E+07	.144E-20	.268E-14	.150E-14	.280E-08	.500E-08
51	.323E+07	.562E-23	.162E-16	.102E-16	.329E-10	.587E-10
52	.562E+07	.110E-25	.618E-19	.346E-19	.194E-12	.347E-12
53	.977E+07	-.100E+01	-.100E+01	.821E-22	.801E-15	-.100E+01

** DIMENSIONAL OUTPUT PARAMETERS **

TIME=	.16942E+00	SEC	.28237E-02 MINUTES	.00 HOURS
NUMBER GEOMETRIC MEAN MASS EQU. RADIUS=	.30123E+00	MICRONS		
MASS MEAN AERODYNAMIC RADIUS=	.22831E+01	MICRONS		
MASS GEOMETRIC MEAN AERODYNAMIC RADIUS=	.17872E+01	MICRONS		
MASS MEDIAN AERODYNAMIC RADIUS=	.18998E+01	MICRONS		
LOGARITHMIC STANDARD DEVIATION=	.20114E+01			
TOTAL PARTICLE NUMBER=	.85342E+07	PARTICLES/C4**3		
TOTAL SUSPENDED MASS=	.21487E+02	G/M**3		

MASS REMOVED BY DIFFUSION=	.34157E-03	GRAMS
MASS REMOVED BY THERMOPHORESIS=	.11361E-01	GRAMS
MASS REMOVED BY SEDIMENTATION=	.33850E+00	GRAMS
MASS REMOVED BY FILTER=	0.	GRAMS
MASS TRAPPED BY LEAK=	.20153E-04	GRAMS
MASS LEAKED FROM CONTAINMENT=	.20190E-04	GRAMS
TOTAL MASS REMOVED=	.35024E+02	GRAMS

INDEX	RADIUS(MICRONS)	RADIUS(MICRONS)	NUMBER(NO./CM**3)	MASS(GRAMS/M**3)	DMASS(GRAMS/M**3)
1	.794E-02	.114E-01	.274E+01	.155E-10	.232E-10
2	.110E-01	.158E-01	.837E+01	.125E-09	.669E-09
3	.132E-01	.190E-01	.293E+02	.750E-09	.407E-08
4	.158E-01	.228E-01	.952E+02	.423E-08	.230E-07
5	.191E-01	.275E-01	.287E+03	.224E-07	.120E-06
6	.229E-01	.330E-01	.803E+03	.109E-06	.585E-06
7	.275E-01	.397E-01	.209E+04	.494E-06	.265E-05
8	.331E-01	.477E-01	.508E+04	.208E-05	.112E-04
9	.398E-01	.574E-01	.115E+05	.813E-05	.439E-04
10	.479E-01	.690E-01	.242E+05	.300E-04	.161E-03
11	.575E-01	.829E-01	.477E+05	.103E-03	.551E-03
12	.692E-01	.997E-01	.878E+05	.329E-03	.176E-02
13	.832E-01	.120E+00	.151E+06	.982E-03	.526E-02
14	.100E+00	.144E+00	.242E+06	.274E-02	.147E-01
15	.120E+00	.173E+00	.364E+06	.715E-02	.383E-01
16	.145E+00	.208E+00	.509E+06	.176E-01	.932E-01
17	.174E+00	.250E+00	.663E+06	.383E-01	.21[illegible]E+00
18	.209E+00	.301E+00	.802E+06	.827E-01	.443E+00
19	.251E+00	.362E+00	.900E+06	.151E+00	.865E+00
20	.302E+00	.435E+00	.935E+06	.231E+00	.156E+01
21	.363E+00	.523E+00	.899E+06	.487E+00	.261E+01
22	.437E+00	.629E+00	.800E+06	.753E+00	.404E+01
23	.525E+00	.756E+00	.660E+06	.108E+01	.578E+01
24	.631E+00	.909E+00	.505E+06	.144[illegible]+01	.769E+01
25	.759E+00	.109E+01	.360E+06	.178E+01	.952E+01
26	.912E+00	.131E+01	.239E+06	.205E+01	.110E+02
27	.110E+01	.158E+01	.148E+06	.226E+01	.119E+02
28	.132E+01	.190E+01	.841E+05	.223E+01	.120E+02
29	.158E+01	.228E+01	.467E+05	.210E+01	.113E+02
30	.191E+01	.275E+01	.237E+05	.185[illegible]+01	.996E+01
31	.229E+01	.330E+01	.113E+05	.153E+01	.822E+01
32	.275E+01	.397E+01	.500E+04	.118E+01	.633E+01
33	.331E+01	.477E+01	.206E+04	.848E+00	.454E+01
34	.398E+01	.574E+01	.795E+03	.567E+00	.304E+01
35	.479E+01	.690E+01	.285E+03	.353E+00	.189E+01
36	.575E+01	.829E+01	.952E+02	.205E+00	.110E+01
37	.692E+01	.997E+01	.296E+02	.111E+00	.594E+00
38	.832E+01	.120E+02	.858E+01	.558E-01	.299E+00
39	.100E+02	.144E+02	.231E+01	.262E-01	.140E+00
40	.120E+02	.173E+02	.582E+00	.114E-01	.613E-01
41	.145E+02	.208E+02	.136E+00	.465E-02	.249E-01
42	.174E+02	.250E+02	.297E-01	.176E-02	.944E-02
43	.209E+02	.301E+02	.602E-02	.621E-03	.333E-02
44	.251E+02	.362E+02	.114E-02	.204E-03	.109E-02
45	.302E+02	.435E+02	.200E-03	.622E-04	.334E-03
46	.363E+02	.523E+02	.327E-04	.177E-04	.948E-04
47	.437E+02	.629E+02	.497E-05	.458E-05	.251E-04
48	.525E+02	.756E+02	.704E-06	.115E-05	.617E-05
49	.631E+02	.909E+02	.926E-07	.253E-06	.141E-05
50	.759E+02	.109E+03	.113E-07	.559E-07	.300E-06
51	.912E+02	.131E+03	.766E-10	.657E-09	.352E-08
52	.110E+03	.158E+03	.261E-12	.385E-11	.208E-10

NRC FORM 335 (7-77)

U.S. NUCLEAR REGULATORY COMMISSION

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13. TYPE OF REPORT
Topical Report

PERIOD COVERED (Inclusive dates)

15. SUPPLEMENTARY NOTES

14. (Leave blank)

16. ABSTRACT (200 words or less)

The QUICK reference computer code for singly contained, single component, aerosol behavior is described. The model equation used is presented and the numerical solution technique -- modified finite difference coupled with the GEAR ordinary differential equation solver -- is discussed briefly. A short description of each subroutine is presented and the logic of the code described in a flow diagram. Input required by QUICK is given in detail, as is the result of a sample run. QUICK is intended to provide a best estimate of aerosol behavior in a homogeneously mixed, nonflowing containment atmosphere. The aerosol particles are assumed to be characterizable by a constant material density, particle mass, a constant dynamic shape factor and a constant collision form factor.

17. KEY WORDS AND DOCUMENT ANALYSIS

17a. DESCRIPTORS

Nuclear Accident Aerosols
Mechanistic Computer Code
Manual

17b. IDENTIFIERS/OPEN-ENDED TERMS

18. AVAILABILITY STATEMENT
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19. SECURITY CLASS (This report)
Unclassified

21. NO. OF PAGES

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22. PRICE
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