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MSPEC Users' Manual

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Battelle Columbus Laboratories

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ABSTRACT

The MSPEC aerosol behavior code for a multiple species, singly contained aerosol 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. Input required by MSPEC is given in detail, as is the result of a sample run. MSPEC is intended to provide a method for estimating aerosol behavior in a homogeneously mixed nonflowing containment atmosphere. The aerosol particles are assumed to be characterizable by representative particles in each of a finite set of size classes. Each representative particle has the average, time varying characteristics of its size class. Large uncertainty rests with the model employed in determining the average shape factors associated with a given size class and composition. This model can, however, be readily modified.

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INTRODUCTION

Present predictions of aerosol behavior in the containment of a nuclear reactor after a severe accident are generally based on the assumption that the aerosol can be treated as an internally homogeneous mixture of the source materials and thus as a single species dispersed phase. Most nuclear aerosol behavior codes, such as HAARM-3[1] and QUICK[2], are thus single species codes.

This situation is unsatisfying because of the suspicion, as yet unconfirmed by experiment, that the single species approximation may break down in some situations such as, for example, those in which particles of different materials are generated at different times and with different size distributions. It was therefore of interest to develop an aerosol behavior model that would be capable of treating a multiple species aerosol typical of nuclear reactor accident conditions.

Research to develop such a model is being sponsored at Battelle by the U.S. NRC and has led to the MSPEC code which is essentially an application of the methods employed in the QUICK code[2] to an aerosol composed of several species. 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 spatially 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 subcompartmentalizes 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.

A second, fundamental assumption is that the expected nonsphericity and fluffiness of the aerosol agglomerates can be modeled using just two correction factors -- the dynamic shape factor and the collision shape factor. These may, however, be functions of particle size and composition. They are treated below.

With these two assumptions, it is possible to set up a system of differential equations for the particle size distribution density analogous to that set up for the QUICK code.[2] However, the necessity to now trace particle composition literally adds another dimension to the problem for each species considered. A full treatment of such a system of equations can be expected to overpower today's computation capacities, and indeed, we were unable to achieve reasonable running times for such a system with just two species.

MSPEC therefore invokes a third, fundamental assumption in order to achieve reasonable computer running times. It is assumed that the dynamic behavior of particles of a given size can be characterized by the properties of a generic particle of that size with average composition. A composition distribution for particles of a given size need therefore not be considered, greatly simplifying the problem. Justification for this simplification must be sought in experimental verification, although it can be shown that, for dynamics that are independent of composition, the assumption is rigorously true.[4]

Given these assumptions, the system of equations used in MSPEC can be developed in close analogy to the discrete system developed for QUICK.[2] Both codes start with the discretization of the particle size parameter -- particle volume, v, is convenient for multi-species systems. It is then assumed that all particles of a volume interval $\Delta v_i = [v_i, v_{i+1}]$ can be characterized by an average volume,

$$\bar{v}_i \equiv (v_i \, v_{i+1})^{\frac{1}{2}} \tag{1}$$

and an average volume fraction, $\bar{X}_{ik}$, for each component k.

The total number of particles on interval Δv_i is approximated by

$$N_i = \int_{v_i}^{v_{i+1}} n(v)dv \sim n(\bar{v}_i)\Delta v_i \tag{2}$$

for an initial or source particle size distribution conveniently read into the code as a continuous density function, $n(v)$. Thereafter, the code deals only in the histogram representation, $\{N_i\}$. Total mass on interval Δv_i is taken as

$$M_i \cong \bar{v}_i \, \bar{\rho}_p \, N_i \tag{3}$$

where $\bar{\rho}_p$ is the average density of particles on the interval. Since, for a continuous initial distribution density,

$$M_i = \bar{\rho}_p \int_{v_i}^{v_{i+1}} n(v) v \, dv \tag{4}$$

$$= \bar{\bar{v}} \, \bar{\rho}_p \int_{v_i}^{v_{i+1}} n(v) \, dv$$

$$\sim \bar{\bar{v}}_i \, \bar{\rho}_p \, N_i,$$

it is clear that a coarse nodal mesh will lead to inconsistency between initial (or source) M_i and N_i unless $\bar{\bar{v}}_i = \bar{v}_i$, which is not generally true. MSPEC uses Equation (3) to derive M_i from N_i and therefore misrepresents the initial or source aerosol mass concentration to some extent for coarse nodal spacing. Using Equation (3) to derive N_i from M_i would lead to a coarse representation of N_i, a situation that may be less desirable because the dynamics of the system depend on N_i rather than M_i.

With the above discretization scheme, the net rate of change of particle volume of species k in volume interval Δv_m due to the various

aerosol behavior mechanisms can be written symbolically as

$$\frac{d}{dt}(\bar{v}_m \bar{X}_{mk} N_m) = \sum_{ij} (DG \bar{Z}_{kij} \bar{v}_m) + S_{mk} \bar{v}_m$$

$$- R_m \bar{v}_m \bar{X}_{mk} N_m - L_m \bar{v}_m \bar{X}_{mk} N_m - F_m \bar{v}_m \bar{X}_{mk} N_m \qquad (5)$$

where R_m is the coefficient for natural removal of particles of volume $\bar{v}_m$ and composition $\{\bar{X}_{mk}\}$, L_m is the leak coefficient, F_m is the filter coefficient, S_{mk} is the number source rate into interval Δv_m for species k and the term $(DG \bar{Z}_{kij} \bar{v}_m)$ is symbolic for net particle volume transport into interval Δv_m by coagulation. The sum, $\sum_{ij}$, symbolizes a summation over all two particle collisions. $G = K_{ij} N_i N_j$ is the collision frequency between particles of interval Δv_i and those of interval Δv_j and D gives the distribution of the resultant particles between intervals Δv_m and Δv_{m+1}, based on the requirement of volume conservation. The fraction D goes to the former interval, the fraction 1-D to the latter. From volume conservation and number accounting in a given collision,

$$D = \frac{\bar{v}_{m+1} - (\bar{v}_i + \bar{v}_j)}{\bar{v}_{m+1} - \bar{v}_m} . \qquad (6)$$

$$\bar{Z}_{kij} = \frac{\bar{X}_{ik} \bar{v}_i + \bar{X}_{jk} \bar{v}_j}{\bar{v}_i + \bar{v}_j} \qquad (7)$$

is the composition of the particle resulting from a collision between a particle from interval Δv_i and one from interval Δv_j.

Equation (5) can be reduced to

$$\frac{d}{dt} N_{mk} = \sum_{ij} (DG \bar{Z}_{kij}) + S_{mk} - R_m N_{mk} - L_m N_{mk} - F_m N_{mk} \qquad (8)$$

by defining $N_{mk} \equiv N_m \bar{X}_{mk}$ and noting that $\bar{v}_m$ cancels out. In this form, it is identical to the equation used in QUICK[2] except for the additional index,

k, and the factor $\bar{Z}_{kij}$ modifying the particle collision rate term. Equation (8) is the fundamental equation of MSPEC.

BEHAVIOR MECHANISMS

The rate coefficients exhibited in Equation (8) above are evaluated on the basis of the characteristic particle of the volume interval of interest from familiar continuum expressions. Thus, if $R(v, \{X_k\})$ is a given removal mechanism, the corresponding discrete term is taken to be

$$R_i = R(\bar{v}_i, \{\bar{X}_{ik}\}) \tag{9}$$

and so on. In the following, the continuum expressions for the various rate coefficients used in MSPEC are presented. Average quantities in these expressions refer to averages over the composition distribution at a given size.

Source Term

This term can be an arbitrary function of time. For convenience, the particle mass distribution on radius is assumed to be log normal, so that only the total mass rate, r_g and σ need be read in for each species to be considered. r_g and σ are assumed to be constant in time.

Natural Removal Terms

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

$$R(v,t) = v_d(v,t)\frac{A_i}{V} \tag{10}$$

where

A_i = Surface area available for deposition due to mechanism i

V = Volume of containment.

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

is given by

$$B(v) = \frac{1}{\bar{\chi} 6\pi\mu r_e} (1+AKn+QKne^{-b/Kn}) \qquad (11)$$

with

$\bar{\chi}$ = Average dynamic shape factor

μ = Viscosity of gas

$r_e = (\frac{3v}{4\pi})^{1/3}$ = Volure equivalent radius

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.[5] Their precise values depend on the particle constituents but do not enter sensitively into typical code predictions.

(i) Sedimentation

For particle Reynolds numbers less than one, the Stokes settling velocity holds.

$$v_d(v,t) = \frac{4\pi}{3} r_e^3 \bar{\rho}_p g\, B(v) \qquad (12)$$

with

$\bar{\rho}_p$ = Average particle material density.

For some severe accident scenarios, however, MSPEC predicts a large fraction of the suspended mass to reside in particles whose diameter exceeds 100 μm. For these, Equation (12) no longer holds and may in fact be off by as much as a factor of two. MSPEC therefore uses empirical data[6] in the form of tables to correct expression (12) for particles whose Reynolds number lies between one and 1259. For Reynolds numbers in excess of 1259, the true settling velocity is easily determined from the fact that the Fanning friction factor is approximately 0.44, independent of Reynolds number.

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

$$fC_F = \frac{F_D}{\pi r_e^2 \bar{\chi}^2 \frac{\rho_g}{2} v_d^2} \qquad (13)$$

where

$\bar{\gamma}$ = Average collision shape factor

C_F = Fanning friction factor for spheres

F_D = Actual drag force on particle.

From the limit requirement that

$$F_D = 6\pi\mu\bar{\chi}r_e v_d \tag{14}$$

and

$$v_d = \frac{2}{9}\,\frac{\bar{\rho}_p g r_e^2}{\mu\bar{\chi}} \tag{15}$$

in the Stokes regime, one can determine f to be equal to $\bar{\chi}/\bar{\gamma}$.

The average collision shape factor, $\bar{\gamma}$, was initially introduced[7] 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: $r_c = \bar{\gamma}r_e$. $\bar{\gamma}$ has never been measured, but approximate values have been inferred by backfitting computer codes. Unfortunately, $\bar{\gamma}$ has also been shown, along with $\bar{\chi}$, to be the most sensitive code parameter.[8]

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

(ii) Diffusion

$$v_d(v,t) = \frac{D(v)}{\delta_D} \tag{16}$$

where

$D(v) = B(v)kT$

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(v) via

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

where

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

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 prediction 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[9], that agrees within a factor of two with available data:

$$F_{\text{thermophoresis}} = \frac{-9\pi\mu^2 r_e \bar{\gamma}}{\rho_g} \phi \frac{\Delta T}{T\delta_{TH}} \qquad (17)$$

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, $\bar{\gamma} r_e$ 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 (17) with data or NaCl aerosol.[10] Measurements on dry Na_2O_2 particles[11] have yielded values of C_t between 1.9 and 2.5, with the former value based on the assumption that $k_g/k_p = 0.001$, the latter on $k_g/k_p = 1.0$. For fluffy agglomerates, the thermal conductivity, k_p, as used in expression (17) probably does not correspond to the particle's material thermal conductivity. It is likely that k_p approaches k_g with increase in 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,

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

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, $\varepsilon_L(v)$, and coefficient

$$L(v,t) = \frac{\dot{V}_L}{V} . \qquad (18)$$

Here

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

The source rate of aerosol number to the environment is

$$[1-\epsilon_L(\bar{v})]N_i \tag{19}$$

for particles in volume interval Δv_i.

Recirculating Filtration

Again, a size dependent filtration efficiency, $\epsilon_F(v)$ is permitted such that

$$F(v,t) = \epsilon_F(v)\,\frac{\dot{V}_F}{V} \tag{20}$$

is the filter coefficient.

Here

$\dot{V}_F$ = 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 MSPEC 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 large scale sodium fire simulation experiments to date, although it appears to be necessary to account for the particle growth observed in some high intensity, small scale experiments.[12]

(i) Brownian Coagulation

$$K(v,v') = 4\pi kT\bar{\gamma}[B(v)+B(v')](r_e+r_e') \tag{21}$$

(ii) Gravitational Coagulation

$$K_G(v,v') = \varepsilon(v,v') \frac{2\pi g \bar{\rho}_p \bar{\gamma}^2}{9\mu\bar{\chi}} \left| r_e^2 - r_e'^2 \right| (r_e + r_e')^2 \qquad (22)$$

where

$\varepsilon(v,v')$ = Collision efficiency.

The collision efficiency can be viewed as that factor which makes expression (22) correct. Most recent experimental and theoretical investigations into this factor[13] have yielded data tables that have been employed in QUICK[2] on large scale sodium fire simulation runs. The results of these runs are surprisingly similar to ones using the simple expression

$$\varepsilon(v,v') = 1.5\left[\frac{\bar{\gamma} r_e}{\bar{\gamma} r_e + \bar{\gamma}' r_e'}\right]^2 \qquad (23)$$

where v', (r_e') refer to the larger particle. Expression (23) strictly holds for inertialess particles and $r_e' >> r_e$ only. Its use for all values of r_e' and r_e yields satisfactory agreement with simulation experiments to date.

(iii) Turbulent Coagulation

An expression for turbulent coagulation was added to MSPEC 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 in most cases of interest.

The two most widely used theoretical treatments of turbulent coagulation are probably those of Saffman and Turner[14] and Levich[15]. 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 MSPEC 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 nonspherical 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 procedure is known for its treatment and none is used in MSPEC. Thus,

$$K_{T+G}(v,v') = 2\sqrt{2\pi}\,\bar{\gamma}^2(r_e+r_e')^2\left[\varepsilon(v,v')^2(\tau_1-\tau_2)^2\frac{1.3E}{\nu}^{3/2}\right. \tag{24}$$

$$\left. + \frac{1}{3}\varepsilon(v,v')^2\,(\tau_1-\tau_2)^2 g^2 + \frac{1}{9}\bar{\gamma}^2(r_e+r_e')^2\frac{E}{\nu}\right]^{1/2}$$

where

$$\tau = \frac{2r_e^2\bar{\rho}_p}{9\bar{\chi}\mu} = \text{Particle response time}$$

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

$$K(v,v') = K_B(v,v') + K_{T+G}(v,v'). \tag{25}$$

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.

Average Values of Particle Density and Shape Factors

The above behavior mechanism expressions contain average values for particle density and shape factors. These averages are indicated by bars above the corresponding symbols and imply averages over the composition distribution of particles in the size interval in question.

The average density of a particle, $\bar{\rho}_{pi}$, can be determined rigorously from

$$\frac{M_i}{\bar{\rho}_{pi}} = \sum_k \frac{M_{ik}}{\rho_k} \tag{26}$$

The average shape factor is less well defined. At best an empirical table would be available that gives both χ and γ as a function of particle size and composition (as well as system thermodynamic state). At present even pure species data are sparse so that an assumption has to be made in the form of a model that gives the derived dependence in tabular or functional form.

The model employed in this version of MSPEC is intuitive and conditional. It has been tested against a single experiment with apparent success but further work is clearly needed, both to determine sensitivity of code prediction to changes in the model and to test the model against experiment.

Interpreting γ as a correspondence factor between a geometric radius, r_g, of a nonspherical particle and its volume equivalent radius, r_e,

$$r_g = \gamma r_e. \tag{27}$$

Volumes are therefore related through

$$v_g = \gamma^3 v_e, \tag{28}$$

and since volumes of the various species composing a given particle are additive, it appears reasonable to attempt a composition model of the form

$$\bar{\gamma}^{-3} = \sum_k X_k \gamma_k^3, \tag{29}$$

where X_k is the volume fraction of species k in the particle. This model is employed for χ as well.

Size dependence of the shape factors is introduced by invoking the work of Kops[16]. He finds, for chain-like, rather than clustered, iron oxide agglomerates that χ is directly proportional to the cube root of the number of primary particles composing the agglomerate -- up to a primary particle number of 5000. Above this value, χ is a constant. MSPEC assumes such a model for all species and assumes that a similar situation pertains to γ. Size dependence of χ and γ is then introduced by varying γ_k (and χ_k) in Equation (29) above linearly with r_e from a value of 1 for r_e equal to the volume average radius of the initial (or source) aerosol of species k, r_{ok}, to the maximum (read in) value when $r_e = 17\ r_{ok}$.

It should be understood that the model outlined above is a first, intuitive approach with little experimental confirmation. Other models are readily conceivable and easily inserted into the code. It can be expected, from the known sensitivity of single species code predictions to values of the shape factors, that the model chosen will significantly influence the results.

Normalization of Model Equation

For numerical reasons, as well as to provide the tools for rigorous scaling of experimental results to full scale reactor containments, Equation (8) is nondimensionalized before being treated by MSPEC. The normalizing dimensions used are a characteristic time associated with Brownian coagulation and mass and length associated with an "average" particle.

The characteristic time for Brownian coagulation is

$$\tau_{BC} = \frac{1}{K_o N_o} \tag{30}$$

where

$$K_o = \frac{2kT}{3\mu}$$

$$N_o = \sum_k N_{ok} + \sum_k SNR_k \cdot \Delta t_{sk} \tag{31}$$

= Total initial and total source potential particle number

N_{ok} = Total initial particle number of species k

SNR_k = Average rate of particle number production of species k over source period Δt_{sk}.

The characteristic mass used is

$$m_o = M_o / N_o \tag{32}$$

where

$$M_o = \sum_k M_{ok} + \sum_k SMR_k \cdot \Delta t_{sk} \tag{33}$$

= Total initial mass and total source potential mass

M_{ok} = Total initial mass of species k

SMR_k = Average rate of particle mass production of species k over source period Δt_{sk}.

Finally the characteristic length used is

$$r_o = \left(\frac{3m_o}{4\pi \bar{\rho}_{p_o}}\right)^{1/3} \tag{34}$$

where $\bar{\rho}_{p_o}$ is the average initial or "potential" source density defined by

$$\frac{M_o}{\bar{\rho}_{p_o}} = \sum_k \frac{M_{ok}}{\rho_k} \tag{35}$$

and ρ_k is the material density of species k.

With these, Equation (8) 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

$$SRBC_k = SNR_k / K_o N_o^2 \tag{36}$$

(ii) Sedimentation

$$GDBC = v_o \frac{A_s}{V} \frac{1}{K_o N_o} \tag{37}$$

where

$$v_o = \frac{2\bar{\rho}_{p_o} g r_o^2}{9\mu}$$

A_s = Surface area available for sedimentation.

(iii) Diffusion

$$DDGD = \frac{kT}{\delta_D g m_o} \frac{A_d}{A_s} \tag{38}$$

where

A_d = Surface area available for diffusion.

(iv) Thermophoresis

$$THGD = \frac{27}{4} \frac{\mu^2}{\rho_g \bar{\rho}_{p_o} g r_o^2} \frac{\Delta T_o}{T} \frac{1}{\delta_{TH}} \frac{A_{TH}}{A_s} \tag{39}$$

where

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

ΔT_o = Arbitrary but characteristic temperature difference, wall/gas, over area A_{TH}. ΔT_o is read in as input.

(v) Leakage

$$VLGD = \frac{\dot{V}_L}{V} \frac{1}{K_o N_o} \frac{1}{GDBC} \tag{40}$$

(vi) Filtration

$$VFGD = \frac{\dot{V}_F}{V} \frac{1}{K_o N_o} \frac{1}{GDBC} \tag{41}$$

(vii) Gravitational Coagulation

$$GCBC = \frac{\pi r_o^2 v_o}{K_o} \tag{42}$$

(viii) Turbulent Coagulation

Motion with fluid

$$TCBC1 = \frac{1}{3} \frac{r_o^3 E^{1/2}}{K_o \nu^{1/2}} \tag{43}$$

Motion relative to fluid

$$TCBC2 = \frac{1.14\, r_o^2 \tau_o E}{K_o \nu^{1/4}}^{3/4} \tag{44}$$

where

$$\tau_o = v_o/g.$$

These eight groups suffice to completely determine the aerosol model MSPEC, once initial conditions are set. They can therefore be used in scaling full scale accident scenarios to experimental scale and vice versa.

Solution of Model Equations

The above describes a generalization of the basic, one species, aerosol behavior equation to a system of ordinary differential equations that describe a multi-species aerosol. This was done in intimate interaction with a scheme for discretizing the basic equation with respect to its particle size dependence -- the MSPEC equations consider discrete particle size classes only.

The resultant system of equations is inherently stiff since the rate coefficients (particularly those of collision processes) are very strong functions of particle size. Under these conditions it is imperative to utilize ordinary differential equation solution techniques designed to treat such systems. MSPEC uses Gear's method as developed by Hindmarsh[17].

BRIEF DESCRIPTION OF SUBROUTINES

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, LEAK, MESH, OUT, RADIUS, SOURCE, XDP) and those used during problem solution (DEPO, DRIVE, EXTEND, KERN, NSTOKE, OUTPUT, RHOSET, REMOVE). Subroutine SSET is recalled at the beginning and end of each aerosol source 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 SOL). The GEAR package is treated as a "black box" by MSPEC.

Input

All input to the MSPEC 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 three 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.

CHIGAM

CHIGAM precalculates the χ and γ values for pure particles of each species. All particles smaller than the average source particle radius for a species are assigned $\chi = \gamma = 1.0$ representing spherical particles. Particles larger than 17 times the average source particle size for a species are

assigned the χ and γ values input for that species. Particles between those sizes are assigned χ and γ values determined by linear interpolation based on equivalent radius. The χ and γ versus size tables determined here are used by RHOSET to calculate the χ and γ values of the composite particles.

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", N_{ik}, 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 last size channel to accumulate the number of particles which grow beyond the range of particle size being considered. The number of size 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.)

The total mass contained in the last size channel is maintained in the last differential equation.

DOUT

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

EXTEND

When coagulation necessitates the inclusion of an additional size 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 to maintain a running total for number and mass lost from the end of the distribution.

FACTORS

The MSPEC 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 2 points is required if an efficiency table is used. The removal rates are used by DEPO and DIFFUN to determine the filter effects.

INIT

Each species in an MSPEC calculation may have an initial log normal distribution. INIT sets up these distributions and determines the number of channels required. INIT calls RHOSET, NSTOKE, KERN, and REMOVE to calculate the coefficients used in the aerosol equations. Size channels which contain more than the fraction BMIN1 of the total aerosol are included in the working range. NS is set equal to the last channel of the working range.

KERN

KERN precalculates the coefficients used in the agglomeration section of DIFFUN. When more than one species is present, KERN is recalled during each iteration to recalculate the coefficients as the characteristics of the particles change with time. The Brownian, gravitational and turbulent coagulation mechanisms are included in KERN. 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 2 points is 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, VDTEMP, VFILTER and VLEAK.

MESH

MESH determines the nodal spacing of the volume channels used by MSPEC. The volume 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 volume.

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. OUT is called by OUTPUT when the IOUT control parameter is 1.

RADIUS

The volume equivalent 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.

RHOSET

RHOSET calculates the average density, χ and γ values for each particle size class. Density is calculated as the inverse of a linear combination of the inverse densities of the species present. The χ and γ values are calculated using a cubic weighting. When more than one species is present RHOSET is called during every iteration.

SETTLE

SETTLE determines the non-Stokesian settling velocities used by NSTOKE. As discussed elsewhere in this report, empirical values of settling velocities are particle Reynolds numbers in excess of one are used. These values are modified to account for the particle shape factors.

SOURCE

SOURCE determines the value of the source coefficients used in the aerosol equation assuming a log normal source particle distribution. SOURCE determines the minimum value of NS for each species which has a source term using BMIN1. It is called by SSET to evaluate the source coefficients at the start of the problem.

SSET

SSET controls the starting and stopping of all sources using the variable TNEXT. When the last source has stopped SSET is deactivated by setting IFLAG=2.

SSLOPE

SSLOPE calculates the variable source mass rate for all species which require a variable source. The slopes calculated here are used by VSOURCE.

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 determines the slope of the cumulative mass curve required by DIFFUN using the table set up by SSLOPE.

XDP

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

OUTPUT

Output from MSPEC is performed 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. In the second section, the dimensional parameters are given since these data are generally in the most useful form. The output from MSPEC is discussed in more detail following the section on the input required for MSPEC.

DESCRIPTION OF INPUT TO MSPEC

A list of the input cards for MSPEC is given in the next section. A detailed description of each input parameter is given below. Input to MSPEC 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	LSTEP	I10	MSPEC 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.
3	DELR	E10.0	Smallest particle radius (micrometers) to be considered by MSPEC. If DELR = 0.0, MSPEC will choose DELR = RGS(M)/(EXP(SIGLS(M))*4), where RGS(M) is the smallest nonzero RGS value input.
4	RMAX	E10.0	Largest particle radius (micrometers) to be considered by MSPEC. There is no maximum value for RMAX.
5	N	I10	Number of channels to be included between DELR and RMAX. MSPEC will add channels as needed up to this number. The maximum value for N is 40, however, most problems work well with $20 < N < 40$. Computer running time is roughly proportional to N^2; however, the smallest recommended value for N is 15. When N is decreased, the mass balance is affected due to the small number of channels available.
6	NF	I10	Number of species to be included. The maximum value is 10. The maximum value for N*NF is 160.
7	DELT	E10.0	Initial time step (seconds) used by the GEAR package. A value of 0.0001 works well.
8	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 $10^{-5} > EPS > 10^{-7}$.

Card No.	Variable Name	Format	Description
9	MF	I10	Determines the solution technique used by the GEAR routine. Use MF = 22 for Gear's method.
10	IOUT	I10	When IOUT = 1, OUTPUT calls the OUT subroutine which displays the derivatives used in the differential equations. Set IOUT = 0 to suppress OUT.
11	ICOMP	I10	ICOMP is used by the OUTPUT to control the printing of the size versus species information. When ICOMP = 0, the mass concentration by size and species is printed. When ICOMP = 1, the mass fraction of each species is printed. When ICOMP = 2, the volume fraction information is shown.
12	ISTOKE	I10	When ISTOKE is zero, the Stokesian settling velocity is used by MSPEC. When ISTOKE is one, a non-Stokesian correction to the settling velocity is used.
13	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.
14	BMIN2	E10.0	The fraction of the total suspended mass which can be lost before MSPEC calls EXTEND. MSPEC 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, MSPEC calls EXTEND to add a channel to the distribution. A recommended range is 10^{-4} to 10^{-5}.
15	T	E10.0	Initial time (seconds).

Card No.	Variable Name	Format	Description
16	TMAX	E10.0	Final time (seconds).
17	ENERGY	E10.0	Turbulent energy dissipation rate density (cm^2/sec^3) in the aerosol system. Set equal to zero to ignore turbulent coagulation. MSPEC makes no provision for time varying turbulence.
18	TENERGY	E10.0	Cut off time (seconds) for turbulent coagulation. TENERGY must be zero when ENERGY = 0.0.
19	PRES	E10.0	Characteristic gas pressure (atmospheres). MSPEC makes no provision for time varying gas pressure.
20	TEMP	E10.0	Characteristic gas temperature (Celsius). MSPEC makes no provision for time varying gas temperature.
21	DTEMP	E10.0	Gas-wall differential temperature (Celsius) used for thermophoretic deposition. If DTEMP > 0.0, Card 4T for NPT must be included.
22	CRATIO	E10.0	Ratio of gas to particle thermal conductivities used for calculation of thermophoretic deposition coefficients.
23	DELD	E10.0	Diffusion boundary layer thickness (cm).
24	DELTH	E10.0	Thermal boundary layer thickness (cm).
25	GEFF	E10.0	Gravitational coagulation collision efficiency. If 0.0 > GEFF > -9.9 $\varepsilon = 1.5(R2/(R1+R2)^2$ is used. If GEFF < -10.0, the GEPS collision efficiency package[13] which is not included with MSPEC is used to calculate the collision efficiency.
26	ASEDV	E10.0	Ratio of sedimentation area to total volume (cm^{-1}).
27	ADIFV	E10.0	Ratio of total internal surface area to total volume (cm^{-1}).
28	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.

Card No.	Variable Name	Format	Description
29	VF	E10.0	Volume fractional flow rate (sec^{-1}) for flow through a recirculating filter. If VF > 0.0 Card 7T for NPVF and Card 10T for NPF must be included.
30	VL	E10.0	Volume fractional leak rate (sec^{-1}) for flow through a leak. If VL > 0.0 Card 13T for NPVL and Card 16T for NPL must be included.
31	VOL	E10.0	Total containment volume (m^3).

Species Parameter Information

After Card 31, the aerosol parameters for each species indicated by NF (Card 6) are contained on a set of three cards (one set per species) described below. Species which have an initial concentration must be input before species which have a source only. Species with a source only must be input in ascending order of the source start time TS1(K).

Card No.	Variable Name	Format	Column Range	Description
1S(K)	SNAME(K)	A10	1-10	Species name, 10 characters maximum.
2S(K)	TMASSI(K)	E10.0	1-10	Total initial mass of this species (g/m^3). TMASSI(K) may be 0.0 if there is no initial concentration.
	RGI(K)	E10.0	11-20	The initial number geometric mean mass equivalent radius of this species (micrometers). Set RGI(K) = 0.0 if TMASSI(K) = 0.0. RGI(K) = $R_{50}(K)/e^{-3\ln^2 SIGI(K)}$
	SIGI(K)	E10.0	21-30	The logarithmic standard deviation of the initial size distribution for species K. It is used with RGI(K) to define the initial log normal distribution for this species. Set SIGI(K) = 0.0 if TMASSI(K) = 0.0. A minimum nonzero value for SIGI(K) of 1.05 is suggested.
3S(K)	RHOS(K)	E10.0	1-10	Particle material density (g/cm^3) of species K.
	CHI(K)	E10.0	11-20	Dynamic shape factor for this species.
	GAMMA(K)	E10.0	21-30	Collision shape factor for this species.
	SMR(K)	E10.0	31-40	Source mass rate (g/m^3 sec) for this species. If this variable is not 0.0, RGS(K) and SIGS(K) must be nonzero.

Card No.	Variable Name	Format	Column Range	Description
3S(K) (Cont'd)	TS1(K)	E10.0	41-50	Source start time for this species (seconds).
	TS2(K)	E10.0	51-60	Source stop time for this species (seconds).
	RGS(K)	E10.0	61-70	The number geometric mean mass equivalent radius (micrometers) of the source distribution for this species. Set RGS(K) = 0.0 if SMR(K) = 0.0.
	SIGS(K)	E10.0	71-80	The logarithmic standard deviation of the source distribution for this species. It is used with RGS(K) to define the source log normal distribution for this species. Set SIGS(K) = 0 if SMR(K) = 0.0. A minimum nonzero value for SIGS(K) of 1.05 is suggested.

After the species parameter cards, the following cards are to be included only when indicated by nonzero values on the indicated input cards. These data specify the input which changes with time or particle size.

Card No.	Variable Name	Format	Condition for Inclusion	Description
1T	NPS(K)	I10	SMR(K) (Card 3S(K)) > 0.0	Number of points for time varying source. NPS(K) can take any integer value from 0 to 20 except 1. A value for NPS(K) is required for every species which has a source.
2T	VSOURCE(NPS,1)	8E10.0	NPS(K) (Card 1T) > 0	Times (seconds) for cumulative source mass.[a]
3T	VSOURCE(NPS,2)	8E10.0	NPS(K) (Card 1T) > 0.0	Cumulative source mass (g/m^3).[a]
4T	NPT	I10	DTEMP (Card 21) > 0.0	Number of points for time varying temperature difference. NPT can take any integer value from 0 to 20 except 1.
5T	VDTEMP(NPT,1)	8E10.0	NPT (Card 4T) > 0	Times (seconds) for temperature difference.[a]
6T	VDTEMP(NPT,2)	8E10.0	NPT (Card 4T) > 0	Gas-wall temperature difference (Celsius).[a] A zero value is assumed at all times outside the range specified on Card 5T.

Card No.	Variable Name	Format	Condition for Inclusion	Description
7T	NPVF	I10	VF (Card 29) > 0	Number of points for variable filter rate. See NPT (Card 4T) for allowed values.
8T	VFIL(NPVF,1)	8E10.0	NPVF (Card 7T) > 0	Times (seconds) for variable filter rate.(a)
9T	VFIL(NPVF,2)	8E10.0	NPVF (Card 7T) > 0	Volume fractional filter flow rate (sec^{-1}).(a) A zero value is assumed at all times outside the range specified on Card 8T.
10T	NPF	I10	VF (Card 29) > 0.0	Number of points for variable filter collection efficiency. See NPT (Card 4T) for allowed values. If NPF = 0 a constant filter efficiency of 1.0 is assumed.
11T	EPSF(NPF,1)	8E10.0	NPF (Card 10T) > 0	Particle radii (micrometers) for variable filter efficiency.(a)
12T	EPSF(NPF,2)	8E10.0	NPF (Card 10T) > 0	Filter collection efficiencies. Allowed values range from 0.0 for no collection to 1.0 for 100% collection.(a) For particles larger than specified on Card 11T, the last efficiency is used.
13T	NPVL	I10	VL (Card 30) > 0.0	Number of points for variable leak rate. See NPT (Card 4T) for allowed values.
14T	VLK(NPVL,1)	8E10.0	NPVL (Card 13T) > 0	Times (seconds) for variable leak rate.(a)
15T	VLK(NPVL.2)	8E10.0	NPVL (Card 13T) > 0	Volume fractional leak flow rates (sec^{-1}).(a) A zero value is assumed for all times outside the range specified on Card 14T.
16T	NPL	I10	VL (Card 30) > 0.0	Number of points for variable leak trapping efficiency. See NPT (Card 4T) for allowed values. If NPL = 0 a constant leak trapping efficiency of 0.0 is assumed.

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

Card No.	Variable Name	Format	Condition for Inclusion	Description
17T	EPSL(NPL,1)	8E10.0	NPL (Card 16T) > 0	Particle radii (micrometers) for variable leak trapping efficiency.(a)
18T	EPSL(NPL,2)	8E10.0	NPL (Card 16T) > 0	Leak trapping efficiency. Allowed values range from 0.0 for no trapping to 1.0 for 100% trapping.(a) For particles larger than specified on Card 17T, the last efficiency is used.

(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 LSTEP	I10	Required	Output interval.
3 DELR	E10.0	Required	Maximum radius (micrometers).
4 RMAX	E10.0	Required	Maximum radius (micrometers).
5 N	I10	Required	Number of channels.
6 NF	I10	Required	Number of species.
7 DELT	E10.0	Required	Initial time step (seconds).
8 EPS	E10.0	Required	Gear routine error criterion.
9 MF	I10	Required	MF = 22.
10 IOUT	I10	Required	OUTPUT calls out when IOUT = 1.
11 ICOMP	I10	Required	Controls display of species information by output.
12 ISTOKE	I10	Required	Specifies non-Stokesian settling when ISTOKE = 1.
13 BMIN1	E10.0	Required	Initial channel cutoff.
14 BMIN2	E10.0	Required	Channel extension criterion.
15 T	E10.0	Required	Initial time (seconds).
16 TMAX	E10.0	Required	Final time (seconds).
17 ENERGY	E10.0	Required	Turbulent energy (cm^2/sec^3).
18 TENERGY	E10.0	Required	Turbulent coagulation cutoff time (seconds).
19 PRES	E10.0	Required	Pressure (atmospheres).
20 TEMP	E10.0	Required	Temperature (Celsius).
21 DTEMP	E10.0	Required	Gas-wall temperature difference (Celsius).
22 CRATIO	E10.0	Required	Ratio gas to particle thermal conductivities.
23 DELD	E10.0	Required	Diffusion boundary layer thickness (cm).
24 DELTH	E10.0	Required	Thermophoretic deposition boundary layer thickness (cm).
25 GEFF	E10.0	Required	Gravitational coagulation collision efficiency.
26 ASEDV	E10.0	Required	Sedimentation area/volume (cm^{-1}).
27 ADIFV	E10.0	Required	Total area/volume (cm^{-1}).
28 ATHV	E10.0	Required	Thermophoretic deposition area/volume (cm^{-1}).
29 VF	E10.0	Required	Volume fraction filtered (sec^{-1}).
30 VL	E10.0	Required	Volume fraction leaked (sec^{-1}).
31 VOL	E10.0	Required	Total volume (m^3).

Species Parameters

After Card 31, a set of three cards is required for each species indicated by NF (Card 6) [species must be input in order of appearance].

Card No.	Variable Name	Format	Column Range	Description
1S(K)	SNAME(K)	A10	1-10	Species name
2S(K)	TMASSI(K)	E10.0	1-10	Initial mass (g/m^3)
	RGI(K)	E10.0	11-20	Initial r_g (micrometers)
	SIGI(K)	E10.0	21-30	Initial σ
3S(K)	RHOS(K)	E10.0	1-10	Material density (g/cm^3)
	CHI(K)	E10.0	11-20	Dynamic shape factor
	GAMMA(K)	E10.0	21-30	Collision shape factor
	SMR(K)	E10.0	31-40	Source mass rate (g/m^3 sec)
	TS1(K)	E10.0	41-50	Source start time (seconds)
	TS2(K)	E10.0	51-60	Source stop time (seconds)
	RGS(K)	E10.0	61-70	Source r_g (micrometers)
	SIGS(K)	E10.0	71-80	Source σ

The next group of cards is used to specify the input parameters which can vary with time or particle size. These cards are included only if the indicated condition is met.

Variable	Format	Condition	Description
1T NPS(K)	I10	SMR(K) > 0.0	Number of points for variable source
2T VSOURCE (NPS,1)	8E10.0	NPS(K) > 0	Variable source times (seconds)
3T VSOURCE (NPS,2)	8E10.0	NPS(K) > 0	Cumulative source mass (g/m^3)
4T NPT	I10	DTEMP > 0.0	Number of points for variable temperature difference
5T VDTEMP (NPT,1)	8E10.0	NPT > 0	Variable temperature difference times (seconds)
6T VDTEMP (NPT,2)	8E10.0	NPT > 0	Gas-wall temperature differences (Celsius)
7T NPVF	I10	VF > 0.0	Number of points for variable filter rate

Variable	Format	Condition	Description
8T VFIL (NPVF,1)	8E10.0	NPVF > 0	Variable filter rate times (seconds)
9T VFIL (NPVF,2)	8E10.0	NPVF > 0	Volume fractional filter flow rates (sec^{-1})
10T NPF	I10	VF > 0.0	Number of points for filter collection efficiency. If NPF = 0 a constant collection efficiency of 1.0 is assumed
11T EPSF (NPF,1)	8E10.0	NPF > 0	Particle radii (micrometers) for filter collection efficiency
12T EPSF (NPF,2)	8E10.0	NPF > 0	Filter collection efficiency
13T NPVL	I10	VL > 0.0	Number of points for variable leak rate
14T VLK (NPVL,1)	8E10.0	NPVL > 0	Variable leak rate times (seconds)
15T VLK (NPVL,2)	8E10.0	NPVL > 0	Volume fractional leak flow rate (sec^{-1})
16T 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.
17T EPSL (NPL,1)	8E10.0	NPL > 0	Particle radii (micrometers) for leak trapping efficiency
18T EPSL (NPL,2)	8E10.0	NPL > 0	Leak trapping efficiency

CODE OUTPUT

The output produced by the MSPEC 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 MSPEC. For a discussion of the nondimensional factors, see the description of the MSPEC model. The printout from OUT comprises several columns showing the channel number, nondimensional volume of the characteristic particle, the nodal spacing on the volume axis, the nondimensional number histogram at the current time and the value and derivative of the dependent variables N_{ik} used in the differential equations.

The output from the MSPEC code OUTPUT routine is described below (see the sample problem output). It can be conveniently divided into two parts: a nondimensional section and a dimensional section in which the MSPEC results are expressed in commonly used units.

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 depositior mechanisms and the total mass removed, all calculated by DEPO, are printed next. The next line shows the nondimensional time, number normalized against NØ and suspended mass normalized against MØ.

The last entries in the nondimensional section are the values in the number and mass bins. MSPEC 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 integration scheme used by DEPO.

The dimensional portion of the output shows the time expressed as seconds, minutes, and hours, followed by several characteristic diameters of the distribution and the standard deviation of the particle distribution. The total number of particles is also shown. The amount of mass suspended and the mass of aerosol removed by each of the deposition mechanisms is printed next by species. The dimensional output shows the particle distribution. The DEQU column shows the volume equivalent diameter for the characteristic particle of each channel. The DGEO column is the geometric diameter (DEQU*γ) for each size class. The DAERO column shows the corresponding aerodynamic diameter. The number and mass columns give the number and mass present in each channel. The composite density and shape factors are also displayed.

When two or more species are present, MSPEC shows the composition of each size class. ICOMP determines whether the masses, mass fractions or volume fractions are displayed. MSPEC shows the composition of the bin channel in the last size class. Since the bin does not have an accurately defined size, no value is printed for DGEO of the bin channel. This section is suppressed when a single species is used (NF = 1).

Error Messages

The most common errors encountered when using MSPEC are caused by invalid input data and breakdown of the solution technique. Input errors are much more common, however. The most common input error is omitting a card or cards because a new option or mechanism is being used. This error is generally detected by the FORTRAN system's input routines. To help identify the missing card(s) MSPEC should be compiled with error traceback. This will make it easier to locate the problem in the input deck.

MSPEC also makes special checks to ensure that the source distribution parameters of a species are input if a source mass rate is given and that the species are entered in the order of their appearance. MSPEC will print an error message and stop execution if not satisfied with the input.

The GEAR ODE package writes its error messages and indications of problems to TAPE 3. The GEAR package returns a negative value of INDEX if it has encountered problems in the solution. MSPEC prints the value of INDEX when a GEAR error has occurred. MSPEC will stop if the GEAR package returns

with three successive errors. The meaning of the GEAR error numbers is shown in Table 1. If errors are reported by the GEAR package, TAPE 3 should be appended to the output file to determine the cause of the error.

TABLE 1. GEAR ERRORS

The GEAR package errors have the following values and meanings:

-1	If integration was halted after failing to pass the error test even after reducing the step size, h, by a factor of 10^{10} from its initial value;
-2	If integration was halted after some initial success either by repeated error test failures or by a direct test indicating that EPS is too small;
-3	If integration was halted after failing to achieve corrector convergence even after reducing h by a factor of 10^{10} from its initial value;
-4	If an input value was found to be illegal; either EPS $\leq$ Ø, N $\leq$ Ø, (TØ-TOUT)*HØ $\geq$ Ø, or the input value of INDEX was illegal.

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* Available for purchase from the NRC/GPO Sales Program, U.S. Nuclear Regulatory Commission, Washington, D.C. 20555, and/or the National Technical Information Service, Springfield, Virginia 22161.

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

SAMPLE PROBLEM OUTPUT

```
MSPEC TEST CASE FOR C/M**3 UO2 AND NA2O2   JUNE 28,1982

** MSPEC AEROSOL BEHAVIOR CODE-MANUAL VERSION = JUNE 22,1982 **

** CODE CONTROL PARAMETERS **

LSTEP                      40
DELE         0.                   MICROMETERS
RMAX          .10000000E+03       MICROMETERS
N                          20
NF                          2
DELT          .10000000E-03
EPS           .10000000E-05
MF                         22
IOUT                        1
ICOMP                       0
ISTOKE                      1
RMIN1         .10000000E-14
RMIN2         .10000000E-04

** DIMENSIONAL INPUT PARAMETERS **

T            0.                   SEC
TMAX          .36000000E+04       SEC
ENERGY       0.                   CM**2/SEC**3
TENERGY      0.                   SEC
PRES          .10000000E+01       ATMOSPHERES
TEMP          .40000000E+02       CELSIUS
DTEMP        0.                   CELSIUS
CRATIO        .10000000E+01
DELD          .10000000E-01       CM
DELTH         .30000000E+00       CM
COEF         -.10000000E+01

ASEDV         .25000000E-03       1/CM
ADIFV         .11000000E-02       1/CM
ATHV          .11000000E-02       1/CM

VF           0.                   VOLUME FRACTION FILTERED/SEC
VL            .11574000E-07       VOLUME FRACTION LEAKED/SEC
VOL           .10000000E+06       CONTAINMENT VOLUME(M**3)
```

**********[illegible] PARAMETERS**********

** K **	1	2
SPECIES NAME	UO2	UN2O2
TMASS(K) (G/(**3)	0.	0.
DGT(K) (MICROMETERS)	0.	0.
SIGI(K)	0.	0.
RHOS(K) (G/C**3)	.1100E+02	.2800E+01
CHT(K)	.3000E+01	.1300E+01
GAMMA(K)	.1500E+02	.5000E+01
SMR(K) (G/MOL)	.2600E-01	.2600E-01
TS1(K) (SEC)	0.	0.
TS2(K) (SEC)	.3600E+04	.3600E+04
DGS(K) (MICROMETERS)	.2000E-01	.2000E+00
SIGS(K)	.1700E+01	.1700E+01

NPS(1) 0 POINTS FOR TIME VARYING SOURCE FOR UO2

NPS(2) 0 POINTS FOR TIME VARYING SOURCE FOR UN2O2

NPVL 0 POINTS FOR VARIABLE LEAK RATE

NPT 0 POINTS FOR TIME TRAPPING EFFICIENCY
A TIME TRAPPING EFFICIENCY OF 0.0 WILL BE ASSUMED

** FUNDAMENTAL GROUPS **

SKRC(1)	SOURCE GROUP	.237[illegible]E-04	RGS(1)	RELATIVE MEDIAN SOURCE RADIUS .3R568R35 /00
SKRC(2)	SOURCE GROUP	.434P43[illegible]E-07	RGS(2)	RELATIVE MEDIAN SOURCE RADIUS .3R568R35E+01
GDRC	GRAVITATIONAL DEPOSITION GROUP	.[illegible]E-08		
DDGD	DIFF[illegible] DEPOSITION GROUP	.[illegible]E+01		
THGC	THERMOPHORETIC DEPOSITION GROUP	0.		
GCRC	GRAVITATIONAL COAGULATION GROUP	.7E6058[illegible]E-04		
TCRC(	TURBULENT COAGULATION GROUP	0.	GRADIENT	
TCRC	TURBULENT COAGULATION GROUP	0.	INERTIA	
VFGC	FILTER FLOW RATE GROUP	0.		
VLGD	[illegible] FLOW RATE GROUP	.35[illegible]E+00		
KN	KNUDSEN NO	.13174731E+01		

NONDIMENSIONALIZED ITEMS

TMAX	.41059405E+05	
TENERGY TURBULENT COAGULATION CUT-OFF	0.	

DIMENSIONAL NORMALIZING PARAMETERS

AVERAGE PARTICLE MASS(XU)	.26071779E-14	GRAMS
AVERAGE PARTICLE RADIUS(RU)	.51853739E-01	MICROMETERS
KU	.15[illegible]E-09	CM**3/SEC
INITIAL PARTICLE NUMBER (N0)	.77374991E+11	PARTICLES/CM**3
CHARACTERISTIC TIME (1/A0*N0)	.86002178E-01	SEC

** DIMENSION OF XUP IS 210 **

INDEX	V	dV	R	RK,RKOUT			
1	.912E-04	.182E-03	.551E-09	.551E-09 ,	.649E-21	.414E-23 ,	.508E-35
2	.458E-03	.968E-03	.600E-07	.609E-07 ,	.254E-19	.373E-19	.162E-31
3	.289E-02	.610E-02	.345E-05	.345E-05 ,	.407E-18	.320E-15 ,	.394E-28
4	.182E-01	.385E-01	.497E-04	.497E-04 ,	.184E-17	.697E-12 ,	.258E-25
5	.115E+00	.243E+00	.193E-03	.193E-03 ,	.206E-17	.406E-09	.455E-23
6	.724E+00	.153E+01	.262E-03	.262E-03 ,	.623E-18	.378E-07 ,	.172E-21
7	.456E+01	.964E+01	.100E-03	.974E-04 ,	.627E-19	.261E-05 ,	.212E-20
8	.288E+02	.608E+02	.427E-04	.251E-04 ,	.308E-19	.176E-04 ,	.402E-20
9	.181E+03	.383E+03	.394E-04	.111E-04 ,	.121E-19	.283E-04 ,	.845E-19
10	.114E+04	.242E+04	.150E-04	.338E-05 ,	-.103E-20	.176E-04 ,	.112E-19
11	.721E+04	.152E+05	.238E-05	.464E-06 ,	-.944E-21	.198E-05 ,	.536E-21
12	.455E+05	.961E+05	.320E-06	.462E-07 ,	-.192E-21	.183E-06 ,	-.120E-20
13	.287E+06	.606E+06	.367E-07	.531E-08 ,	-.295E-22	.209E-07	.303E-21
14	.181E+07	.382E+07	.398E-08	.606E-09 ,	-.367E-23	.238E-08 ,	-.494E-22
15	.114E+08	.241E+08	.368E-09	.746E-10 ,	.190E-23	.293E-09 ,	-.163E-23
16	.719E+08	.152E+09	.529E-10	.107E-10 ,	-.117E-23	.421E-10 ,	.437E-24
17	.453E+09	.957E+09	.923E-11	.167E-11 ,	.185E-24	.656E-11 ,	-.192E-25

15	.2[illegible]E+10	.[illegible]E+10	.129E-11	.261E-12 ,	-.208E-25	.103E-11 ,	.224E-24
19	.1[illegible]E+11	.[illegible]E+11	.256E-13	.519E-13 ,	-.331E-25	.204E-12 ,	-.148E-25
20	.1[illegible]E+12	.2[illegible]E+12	.116E-11	.827E-12 ,	.215E-16	.333E-11 ,	.844E-16

[illegible] [illegible] 1434

** [illegible] OUTPUT **

[illegible] .2[illegible]E+04

MASS REMOVED BY DIFFUSION= .[illegible]E-05
MASS REMOVED BY THERMOPHORESIS= 0.
MASS REMOVED BY SEDIMENTATION= .504E+00
MASS REMOVED BY FILTER= 0.
MASS TRAPPED BY LEAK= 0.
MASS LEFT IN CHEM CONTAINMENT= .362E-03
TOTAL MASS REMOVED= .504E+00

TIME= .[illegible]E+03 NUMBER= .709E-03 RADS= .905E-01

NUMBER LOST FROM DISTRIBUTION = .416E-11
MASS LOST FROM DISTRIBUTION = .451E+00

** DIMENSIONAL OUTPUT **

TIME= .360[illegible]E+04 SEC .60000E+02 MINUTES 1.00 HOURS

NUMBER GEOMETRIC MEAN MASS DIA. DIAMETER= .995[illegible]E-01 MICRONS
MASS MEAN AERODYNAMIC DIAMETER= .431[illegible]E+02 MICRONS
MASS GEOMETRIC MEAN AERODYNAMIC DIAMETER= .[illegible]E+01 MICRONS
MASS [illegible] AERODYNAMIC DIAMETER= .[illegible]E+01 MICRONS
LOGARITHMIC STANDARD DEVIATION= .[illegible]E+01
TOTAL PARTICLE NUMBER= .54813E+08 PARTICLES/CM**3

** AIRBORNE, REMOVED AND REMAINING QUANTITIES **

SPECIES	AIRBORNE	DIFFUSION	THERMOPHORESIS	REMOVED BY SEDIMENTATION	FILTER	LEAK	TRAPPED BY LEAK
[illegible]	.[illegible]E+06	.7[illegible]E+02	0.	.[illegible]E+07	0.	.383[illegible]E+02	0.
[illegible]	.[illegible]E+06	.7[illegible]E+02	0.	.[illegible]E+07	0.	.346[illegible]E+02	0.
TOTAL	.[illegible]E+07	.[illegible]E+02	0.	.[illegible]E+08	0.	.730[illegible]E+02	0.
TOTAL REMAINING				.[illegible]E+08			

INDEX	DIAMETER(CENTIMETERS)	DIAMETER(METERS)	DIAMETER(MICRONS)	NUMBER/CU.M. /CM**3)	MASS(GRAMS/M**3)	RHO	CHI	GAMMA
1	.[illegible]	.[illegible]	.155E-01	.426E+02	.250E-10	11.0	1.0	1.0
2	.[illegible]	.[illegible]	.276E-01	.471E+04	.139E-07	11.0	1.0	1.0
3	.1[illegible]	.1[illegible]	.[illegible]	.[illegible]	.[illegible]	11.0	1.0	1.0
4	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.449E-03	11.0	1.0	1.0
5	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.110E-01	11.0	1.0	1.1
6	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.941E-01	11.0	1.1	1.9
7	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.227E+00	10.8	1.3	3.4
8	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.423E+00	7.6	1.5	5.2
9	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.[illegible]	5.1	1.7	7.4
10	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.374E+01	4.5	1.9	8.9
11	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.338E+01	4.4	1.8	8.8
12	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.209E+01	4.5	1.9	8.9
13	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.151E+01	4.5	1.9	9.1
14	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.109E+01	4.5	1.9	9.2
15	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.[illegible]	4.5	1.9	9.2
16	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.765E+00	4.5	1.9	9.2
17	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.751E+00	4.5	1.9	9.2
18	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.741E+00	4.5	1.9	9.2
19	.[illegible]	.[illegible]	.[illegible]	.[illegible]	.928E+00	4.5	1.9	9.2

MASS (G/M**3)

INDEX	DIAMETER(CENTIMETERS)	H2O	N2O4
1	.[illegible]	.250E-10	.[illegible]
2	.[illegible]	.[illegible]	.[illegible]
3	.1[illegible]	.995E-05	.[illegible]
4	.[illegible]	.449E-03	.[illegible]
5	.[illegible]	.110E-01	.[illegible]
6	.[illegible]	.941E-01	.[illegible]
7	.[illegible]	.227E+00	.[illegible]
8	.[illegible]	.[illegible]	.[illegible]
9	.[illegible]	.997E+00	.[illegible]
10	.[illegible]	.192E+01	.[illegible]
11	.[illegible]	.166E+01	.[illegible]
12	.[illegible]	.104E+01	.[illegible]
13	.[illegible]	.757E+00	.[illegible]
14	.[illegible]	.[illegible]	.[illegible]
15	.[illegible]	.423E+00	.[illegible]
16	.[illegible]	.382E+00	.[illegible]
17	.[illegible]	.376E+00	.[illegible]
18	.[illegible]	.371E+00	.[illegible]
19	.[illegible]	.464E+00	.[illegible]
20	[illegible]	.444E+02	.[illegible]

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16. ABSTRACT (200 words or less)

The MSPEC aerosol behavior code for a multiple species, singly contained aerosol 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. Input required by MSPEC is given in detail, as is the result of a sample run. MSPEC is intended to provide a method for estimating aerosol behavior in a homogeneously mixed nonflowing containment atmosphere. The aerosol particles are assumed to be characterizable by representative particles in each of a finite set of size classes. Each representative particle has the average, time varying characteristics of its size class. Large uncertainty rests with the model employed in determining the shape factors associated with a given size class and composition. This model can, however, be readily modified.

17. KEY WORDS AND DOCUMENT ANALYSIS

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