**PLUVIUS: A Generalized
One-Dimensional Model of
Reactive Pollutant Behavior,
Including Dry Deposition,
Precipitation Formation, and
Wet Removal**

Second Edition

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November 1984

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PREFACE

This second-edition user's manual describes Mod 5.0, the most recent version of the one-dimensional "PLUVIUS" reactive-storm simulation code. Mod 3.1, a predecessor, was documented in the original PLUVIUS manual (Hales, 1981) approximately two years prior to this writing, and has been used rather extensively since that time. Our operating experience with Mod 3.1 during this period has led to a progressive series of improvements which have been collectively implemented in Mod 5.0, and it is appropriate at this point to document these advances for the general user community. The most important of these changes are itemized as follows:

- The numerical integration scheme has been changed to utilize cubic-spline spatial differencing. This differs from Mod 3.1, which employs a generalized Crank-Nicholson technique. Temporal differencing in Mod 5.0 continues to apply a conventional Crank-Nicholson approach. This modification has substantially improved the accuracy and computational efficiency of the code. More importantly, however, it has removed an instability problem which was frequently observed with Mod 3.1 under high precipitation conditions. Termed a "static" instability by Roach (1972), this is a potential problem whenever advection terms are represented by space-centered differences. The fourth-order spline technique employed by Mod 5.0 avoids this type of differencing and thus eliminates this particular source of instability.
- An operator-splitting technique is employed with Mod 5.0, which segregates transport and reaction terms. The primary advantage of this modification lies in Mod 5.0's enhanced ability to deal with rapidly-reacting and near-equilibrium systems. Integration of reaction terms is performed using a standard/stiff code for ordinary differential equations.
- Although we refer to PLUVIUS as a one-dimensional model, it may also be used for some two-dimensional, steady-state applications. For the case where the horizontal wind speed is independent of height, the difference between the one-dimensional time-dependent problem and

two-dimensional steady-state problem is merely a change in the frame of reference. An enhancement in Mod 5.0 allows the modeling of two-dimensional steady-state situations with wind shear--a case that cannot be treated in the one-dimensional mode.

- Some basic improvements have been made in the code's energy-balance formulation, and in the numerical procedure with which the energy balance is computed.
- A more convenient bookkeeping procedure has been implemented for problem set-up and for dealing with multiple reactive species.

In addition to the above modifications to the code itself, we have provided a refined example problem, which includes more elegant characterizations of cloud-physical processes than those given in its Mod 3.1 counterpart. The chemistry in this example is also somewhat more detailed, but has been kept sufficiently simple to avoid obscuration of salient points of the code. The user can, of course, modify and extend this example at will, depending upon his individual needs.

Mod 5.0 is a substantial improvement over its predecessor, in the sense that it is more versatile, more efficient, more accurate, and easier to use. Although this strongly implies the obsolescence of Mod 3.1, it should not be taken to suggest immediate replacement of this older code in all cases. For current, limited applications where Mod 3.1 is performing satisfactorily, the user may be well-advised to continue with his on-line code. For new or anticipated extensive uses, however, one definitely should select this later and significantly improved version.

We expect that this second-edition manual will be the last user's guide published for the one-dimensional PLUVIUS series. Our newer multi- (1, 2, or 3) dimensional "PLUVIUS II" code has recently become operational, and we anticipate that this more versatile code will be documented in user's-manual form in the future, after more substantial operation experience has been obtained.

This research has been funded as part of the National Acid Precipitation Assessment Program by the U.S. Environmental Protection Agency. We sincerely thank the EPA and the American taxpayer, who have acted jointly to make this effort possible.

ABSTRACT

This report is a second-edition user's manual for the PLUVIUS reactive-storm model. The PLUVIUS code simulates the formation of storm systems of a variety of types, and characterizes the behavior of air pollutants as they flow through, react within, and are scavenged by the storms.

The computer code supplied with this report is known as PLUVIUS MOD 5.0, and is a substantial improvement over the MOD 3.1 version given in the original user's manual. Example applications of MOD 5.0 are given in the report to facilitate rapid application of the code for a variety of specific uses.

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-Man is not capable of thought in any high degree, and even the most spiritual and highly cultivated of men habitually sees the world and himself through the lenses of delusive formulas and artless simplifications.

Hermann Hesse, *Steppenwolf*

1. INTRODUCTION

During recent years numerous investigations of atmospheric behavior have been performed using one-dimensional simplifications of the continuity equations for mass, energy, and momentum. Such methods necessarily sacrifice some aspects of reality in the context of our three-dimensional atmosphere; but quite often they lead to valuable insights which could not be obtained otherwise within the constraints of computational capabilities and human perception. In the context of the Steppenwolf's rather pessimistic observation, one-dimensional models (and indeed all other types of atmospheric interpretive models) create a type of lens through which atmospheric processes can be observed. They are imperfect lenses; but frequently they are capable of creating insights and concepts which would be largely impossible in their absence.

This statement is certainly a valid one with reference to air-pollutant transformation and removal processes. The chemistry and physics of these phenomena tend to be both poorly understood and mathematically complex, and the computational simplicity of one-dimensional modeling is thus a highly attractive feature. One example of such an application is the analysis of Omstedt and Rodhe (1978), who performed computations for the three-component system $\text{H}_2\text{S}-\text{SO}_2-\text{SO}_4^-$ using various assumptions with regard to chemical reaction, deposition and vertical transport.

Previous computer codes applied for these purposes tend to be rather specific to the immediate requirements at hand, and it seems desirable to possess a generalized code which would provide a flexible framework for numerous types of calculations. Specifically, there is a need for a code which would allow for:

- variable diffusion in height and time
- generalized boundary conditions at both the top and bottom of the computational grid, allowing a versatile characterization of the deposition/resuspension process
- flexible vertical grid spacing
- the capability to describe cloud and precipitation formation phenomena
- the versatile incorporation of aqueous-phase and gaseous-phase chemical conversion for multiple-component systems, and
- the capability to describe wet removal processes.

The present report describes a code which has been developed for this purpose, and the following chapters provide a user's manual for its practical application. This manual begins by formulating the one-dimensional conservation equations to be used by the code. It then gives an overview of the code, which is intended to facilitate its use for example calculations, which constitute the final portion of the main body of the report. More detailed description of the code, along with a discussion of its numerical procedures, is given in the Appendices.

2. FORMULATION OF GOVERNING EQUATIONS AND BOUNDARY CONDITIONS^(a)

A. GOVERNING EQUATIONS DESCRIBING MATERIAL-BALANCE RELATIONSHIPS

The starting point for this derivation is the conventional continuity equation for pollutant species k (cf. Bird, Stewart, and Lightfoot, 1960):

$$\frac{\partial c_k}{\partial t} = - \nabla \cdot (c_k \mathbf{v}_k) + G_k \quad (1)$$

$$k = 1, 2, 3, \dots, m$$

where c denotes molar concentration, $\mathbf{v}_k$ is the pollutant velocity vector and G is a volumetric generation term. Dropping the subscript k for convenience, applying conventional K-theory treatment, and expanding the divergence term yields the form

$$\frac{\partial c}{\partial t} = - \frac{\partial}{\partial x} (cu) - \frac{\partial}{\partial y} (cv) - \frac{\partial}{\partial z} (cw) + \nabla \cdot \mathbf{F} + G \quad (2)$$

u , v , and w are the nondiffusive x , y , and z components of the individual pollutant velocities, and $\mathbf{F}$ is the pollutant flux arising from turbulent transport.

Let the corresponding components of air velocity be u_A , v_A , and w_A , and assume that

$$u = u_A \quad (3)$$

and
$$v = v_A$$

(a) The mathematics of this section are somewhat involved, and it is suggested that the reader skim this material initially and proceed rapidly to later sections describing code use. This section can be re-studied as necessary after the user has had initial experience executing the code.

Also let $w = w_A + w_r$ (4)

where w_r represents the "settling" velocity of the pollutant species.

The following approximations are now applied:

- Because only one-dimensional or two-dimensional systems will be considered, neglect all variation with y .

Let c^* represent the molar concentration of air, and neglect horizontal and temporal variations in c^* , so that the continuity equation for air becomes

$$c^* \left(\frac{\partial u_A}{\partial x} + \frac{\partial w_A}{\partial z} \right) + w_A \frac{\partial c^*}{\partial z} = 0 \quad (5)$$

- Ignore the horizontal component of the turbulent transport and apply the gradient-transport approximation, so that

$$\nabla \cdot \mathbf{F} = \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] \quad (6)$$

where D_m is the eddy diffusion coefficient.

The species continuity equation [Equation (2)] now becomes:

$$\begin{aligned} \frac{\partial c}{\partial t} = & - u_A \frac{\partial c}{\partial x} - w_A \frac{\partial c}{\partial z} - \frac{\partial}{\partial z} (w_r c) \\ & + \frac{c}{c^*} w_A \frac{\partial c^*}{\partial z} + \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] + G \end{aligned} \quad (7)$$

At this point the development separates for the one-dimensional, time-dependent, and two-dimensional, steady-state cases. In the one-dimensional case one assumes that the horizontal air speed is constant with height, and proceeds to express the vertical air velocity as the sum of the change rate of terrain elevation w_{A0} and some additional component w'_A ; i.e.,

$$w_A = w_{A0} + w'_A \quad (8)$$

Defining in addition a "terrain-following" derivative

$$\frac{\hat{D}c}{\hat{D}t} = \frac{\partial c}{\partial t} + w_{Ao} \frac{\partial c}{\partial z} + u_A \frac{\partial c}{\partial x} , \quad (9)$$

Equation (7) can be expressed by the form

$$\begin{aligned} \frac{\hat{D}c}{\hat{D}t} = & - \frac{\partial}{\partial z} \left[(w_r + w_A') c \right] + \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] + c \frac{\partial w_A'}{\partial z} \\ & + c \frac{w_A}{c^*} \frac{\partial c^*}{\partial z} + G \end{aligned} \quad (10)$$

Here the total derivative $\hat{D}c/\hat{D}t$ can be visualized as the time rate of change of material in a vertical column of air moving with the velocity u_A , v_A , w_{Ao} . G is a catch-all term, providing for the combined effects of reaction and interphase transport.

For the two-dimensional, steady-state case one assigns the term u_{Ao} to describe u_A at the surface (the bottom level of the model domain), and defines u^* as the horizontal velocity at some chosen reference level. Partitioning the vertical velocity by

$$w_A = w_{Ao} (u_A/u_{Ao}) + w_A'' , \quad (11)$$

and defining a new derivative

$$\frac{D^*c}{Dt^*} = u^* \frac{\partial c}{\partial x} + (u^*/u_{Ao}) w_{Ao} \frac{\partial c}{\partial z} , \quad (12)$$

Equation (7) becomes

$$\begin{aligned} \frac{D^*c}{Dt^*} = & \frac{u^*}{u_A} \left\{ - \frac{\partial}{\partial z} \left[(w_r + w_A'') c \right] + \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] \right. \\ & \left. + c \frac{\partial w_A''}{\partial z} + c \frac{w_A}{c^*} \frac{\partial c^*}{\partial z} + G \right\} \end{aligned} \quad (13)$$

Under conditions when u_A is constant with height, $u_A = u^*$ and Equation (13) is identical to Equation (10). When u_A is not constant, the physical interpretations of Equations (10) and (13) differ. In Equation (10), $\hat{D}c/\hat{D}t$ represents the rate of change in a vertical column moving with the horizontal velocity of the air. Thus the column maintains a physical integrity. In Equation (13), D^*c/Dt^* also represents the rate of change in a vertical column, but in this case the column is moving at the velocity u^* and air is flowing horizontally through the column at all levels where $u_A \neq u^*$. The column at some time t^* corresponds to a column at position x , where

$$x = x_0 + u^* (t^* - t_0^*) ,$$

and air at different levels may take different physical times to move from x_0 to x . Conveniently, Equations (10) and (13) have similar mathematical forms, so the same code can be used to provide solutions for both situations. An important restriction on the use of Equation (13) is that u_A must be either always positive or always negative. Physically, this means that situations with flow moving in opposite directions at different levels cannot be handled; this restriction is imposed by the "forward-marching" technique used in PLUVIUS' numerical integration scheme.

It is important to note that PLUVIUS is not a dynamical model. Thus, the air velocity components u_A and w_A are not calculated internally, but must be provided by the user in the form of some sort of "driver." Input wind data can be derived from actual measurements, from some dynamical atmospheric model, or even from some hypothetical test simulation. In any case, it is the user's responsibility to provide physically realistic values, as the model accepts them rather blindly. In particular, the mass continuity equation [Equation (5)] should be satisfied.

B. INITIAL AND BOUNDARY CONDITIONS FOR MATERIAL-BALANCE RELATIONSHIPS

Equations (10) and (13) are second-order parabolic with two independent variables, and as such they require two boundary conditions and

one initial condition for a complete formulation of the problem. The initial condition can be stated quite simply as

$$c(0,z) = \hat{c}_I(z) \quad (14)$$

where $\hat{c}_I$ is some specified initial concentration field.

Boundary conditions must be specified at the top ($z = h$) and bottom ($z = 0$) of the model domain. Three forms chosen for the present application correspond to the so-called "inflow," "outflow," and "flux" conditions.

The inflow condition represents a situation where at the boundary, the species has a net velocity into the model domain. This net velocity is $w_r + w_A'$, but we have placed the restriction that $w_A' = 0$ at the two boundaries (there is no flow of air through the boundaries), so the net velocity reduces to w_r . Physically, the inflow condition is appropriate at the top boundary for species with a significant settling velocity. The condition is implemented by specifying the concentration at the boundary. Thus, at the top,

$$c(t,h) = \hat{c}_T(t) \quad , \quad (15)$$

and at the bottom,

$$c(t,0) = \hat{c}_B(t) \quad , \quad (16)$$

where $\hat{c}_T$ and $\hat{c}_B$ are specified concentrations.

The outflow condition is the opposite to the inflow condition. It is particularly appropriate at the bottom boundary for species having a significant settling velocity, such as precipitation particles, or pollutants in precipitation particles. The condition is actually a computational condition, representing the fact that the outflow concentration is generated "upstream" within the model domain. It is discussed more fully in Appendix A. It should be noted that the outflow boundary condition has only been implemented at the bottom boundary in PLUVIUS.

The flux boundary condition represents a situation where the boundary acts as an impermeable or semipermeable barrier, and any transport occurring across the boundary is influenced by processes outside of the model's domain. Examples are dry deposition of gases and submicron particles, and moisture transfer from evaporation and condensation. Mathematically, the condition is expressed as

$$\left[w_r c - D_m c^* \frac{\partial}{\partial z} \frac{c}{c^*} \right] \Big|_{t,h} = \hat{f}_T(t) \quad (17)$$

$$\text{and} \quad \left[w_r c - D_m c^* \frac{\partial}{\partial z} \frac{c}{c^*} \right] \Big|_{t,0} = \hat{f}_B(0) \quad , \quad (18)$$

where $\hat{f}_T$ and $\hat{f}_B$ are the specified fluxes at the top and bottom boundaries, respectively (units = moles/cm² sec). As an example, an impermeable boundary is specified by $\hat{f}_T = 0$ or $\hat{f}_B = 0$. An example for dry deposition is given in Section 5.

C. GOVERNING EQUATION DESCRIBING ENERGY-BALANCE RELATIONSHIP

It is important to note that energy-balance considerations are necessary to the current model only when one desires to compute temperature distributions within the atmosphere. In view of this the following formulation is unnecessary for many applications; and indeed the model's computer code allows the associated operations to be bypassed when appropriate.

The starting point for formulation of the appropriate energy-balance equation can be obtained from Equation (10.1-19) from Bird, Stewart, and Lightfoot (1960). Expressing this equation on a molar basis, neglecting viscous generation, and adding a latent-heat term one obtains the form

$$c^* C_v \frac{DT}{Dt} = -\nabla \cdot \mathbf{q} - T \left(\frac{\partial p}{\partial T} \right)_v \nabla \cdot \mathbf{y}_A + \dot{H} \quad , \quad (19)$$

where

C_v = specific heat of air at constant volume (molar basis)

T = air temperature

$$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + \mathbf{v}_A \cdot \nabla T$$

$\mathbf{q}$ = sensible heat flux vector

p = pressure

$\hat{v}$ = specific volume

$\mathbf{v}_A$ = three-dimensional air-velocity vector

and $\dot{H}$ = energy generation rate per unit volume from latent heating effects.

The second term on the right of Equation (19) may be converted to a more tractable form using the ideal-gas law and the continuity equation. From the ideal-gas law,

$$\left(\frac{\partial p}{\partial T} \right)_{\hat{v}} = R c^* \quad (20)$$

where R is the gas constant. In addition, one can combine the gas law with the continuity equation to obtain

$$\nabla \cdot \mathbf{v}_A = \frac{1}{T} \frac{DT}{Dt} - \frac{1}{p} \frac{Dp}{Dt} \quad (21)$$

Assuming that the substantial derivative of p is dominated by the vertical advection term, and invoking the hydrostatic assumption one obtains

$$\frac{1}{p} \frac{Dp}{Dt} \cong \frac{w_A}{p} \frac{\partial p}{\partial z} \cong -w_A \frac{g m_a}{RT} \quad (22)$$

where m_a is the mean molecular weight of air and g is the gravitational acceleration. Equations (20), (21), and (22) now can be combined to provide the useful form

$$T \left(\frac{\partial p}{\partial T} \right) \hat{\nabla} \cdot \mathbf{y}_A = R c^* \frac{DT}{Dt} + w_A c^* g m_a \quad . \quad (23)$$

For the sensible heat flux, we apply gradient-transport theory, and again assume that the vertical component dominates, so that

$$- \nabla \cdot \mathbf{q} = \frac{\partial}{\partial z} \left[c^* c_p D_H \left(\frac{\partial T}{\partial z} - \Gamma_d \right) \right] \quad (24)$$

where Γ_d is the dry adiabatic lapse rate,

$$\Gamma_d = - g m_a / c_p \quad , \quad (25)$$

and

$$c_p = c_v + R \quad (26)$$

Substitution of Equations (23), (24), (25) and (26) into Equation (19) yields

$$\frac{DT}{Dt} = w_A \Gamma_d + \frac{1}{c^*} \frac{\partial}{\partial z} \left[c^* D_H \left(\frac{\partial T}{\partial z} - \Gamma_d \right) \right] + \frac{\dot{H}}{c^* c_p} \quad . \quad (27)$$

Equation (27) can be considered as the basic form of the energy balance to be applied in PLUVIUS, although the functional form of the latent-heating term $\dot{H}$ remains to be specified. Under conditions where cloud and precipitation particles are present, $\dot{H}$ can be of major importance in the equation. This term represents a variety of transfer processes between water vapor and liquid and solid particles of numerous shapes and sizes. In general one may write

$$\dot{H} = L_c G_{vl} + L_f G_{ls} + (L_c + L_f) G_{vs} \quad (28)$$

where

L_c = latent heat of condensation (ergs/mole)

L_f = latent heat of fusion (ergs/mole)

G_{vl} = net rate of transfer of water from vapor to liquid particles
(moles/cm³sec)

$G_{\ell s}$ = net rate of transfer of water from liquid to solid particles

G_{vs} = net rate of transfer of water from vapor to solid particles.

Under subsaturated conditions we shall apply variants of equation (27) directly in the model, incorporating latent-heating effects as an explicit add-on term (Equation 28) as indicated. Under saturated conditions, however, we shall assume that a near-equilibrium exists between cloud water and water vapor; and because of this assumption it is expedient to incorporate the associated heating terms implicitly within the calculation, rather than as explicit rate components. To produce this semi-implicit formulation we define the saturation mixing ratio for water vapor, r_{vs} , as

$$r_{vs} = \frac{c_{vs}}{c^*} = \frac{e_s}{p} \quad (29)$$

where c_{vs} is the saturation vapor density for water (mole/cm³) and e_s is the saturation vapor pressure. A mass-balance equation can be written for r_{vs} , which combines Equation (7) for c_{vs} and c^* , as

$$c^* \frac{Dr_{vs}}{Dt} = \frac{\partial}{\partial z} \left[c^* D_z \frac{\partial r_{vs}}{\partial z} \right] + G_{v\ell} + G_{vs} \quad (30)$$

It is important to note that Equation (30) is valid only at conditions of saturation equilibrium, while a similar equation for r_v , the (not necessarily saturated) water-vapor mixing ratio, will always hold.

e_s is strictly a function of T , and can be expressed in terms of the Clausius-Clapeyron equation as

$$\frac{de_s}{dT} = \frac{e_s L_c}{RT^2}, \quad (31)$$

so that

$$\frac{\partial r_{vs}}{\partial \xi} = r_{vs} \left[\frac{L_c}{RT^2} \frac{\partial T}{\partial \xi} - \frac{1}{p} \frac{\partial p}{\partial \xi} \right] \quad (32)$$

where ξ is any of the independent variables (x,y,z,t).

Equation (28) can be rearranged as follows:

$$G_{vl} + G_{vs} = \frac{\dot{H}}{L_c} - \frac{L_f}{L_c} G_{ls} - \frac{L_f}{L_c} G_{vs} \quad (28')$$

Under the assumption that $D_z \approx D_H$, this can be combined with Equations (27) and (30) to yield

$$\frac{DT}{Dt} = w_A \Gamma_w + \frac{1}{c^* x_1} \frac{\partial}{\partial z} \left[c^* x_1 D_H \left(\frac{\partial T}{\partial z} - \Gamma_w \right) \right] + \frac{\dot{H}_w}{c^* x_1 c_p} \quad (33)$$

where

$\Gamma_w = \Gamma_d x_2/x_1$ is the wet adiabatic lapse rate,

$$x_2 = 1 + L_c r_{vs}/RT,$$

$$x_1 = 1 + L_c^2 r_{vs}/c_p RT^2,$$

$$\dot{H}_w = L_f (G_{ls} + G_{vs}).$$

Noting the similar forms of Equations (27) and (33), we will write

$$\frac{DT}{Dt} = w_A \Gamma + \frac{1}{c^* \chi} \frac{\partial}{\partial z} \left[c^* \chi D_H \left(\frac{\partial T}{\partial z} - \Gamma \right) \right] + \frac{\dot{H}^*}{c^* \chi c_p} \quad (34)$$

where for unsaturated conditions,

$$\Gamma = \Gamma_d$$

$$\chi = 1$$

$$\dot{H}^* = \dot{H}$$

and for saturated conditions,

$$\Gamma = \Gamma_w$$

$$\chi = \chi_1$$

$$\dot{H}^* = \dot{H}_w$$

All that remains now is to put Equation (34) in a form suitable for our one-dimensional and two-dimensional steady-state conditions. For the one-dimensional case, Equation (34) becomes

$$\begin{aligned} \frac{\hat{D}T}{\hat{D}t} = & - \frac{\partial}{\partial z} (w_A' T) + \frac{1}{c^* \chi} \frac{\partial}{\partial z} \left[c^* \chi D_H \frac{\partial T}{\partial z} \right] \\ & + T \frac{\partial w_A'}{\partial z} + w_A \Gamma - \frac{1}{c^* \chi} \frac{\partial}{\partial z} (c^* \chi D_H \Gamma) + \frac{\dot{H}^*}{c^* \chi C_p} \end{aligned} \quad (35)$$

For the two-dimensional, steady-state case, Equation (33) becomes

$$\begin{aligned} \frac{D^*T}{Dt^*} = & \frac{u^*}{u_A} \left\{ - \frac{\partial}{\partial z} (w_A'' T) + \frac{1}{c^* \chi} \frac{\partial}{\partial z} \left[c^* \chi D_H \frac{\partial T}{\partial z} \right] \right. \\ & \left. + T \frac{\partial w_A''}{\partial z} + w_A \Gamma - \frac{1}{c^* \chi} \frac{\partial}{\partial z} (c^* \chi D_H \Gamma) + \frac{\dot{H}^*}{c^* \chi C_p} \right\} \end{aligned} \quad (36)$$

These two equations are substantially similar in form to Equations (10) and (13), and basically the same solution technique is used for the energy and mass balance equations.

D. INITIAL AND BOUNDARY CONDITIONS FOR THE ENERGY-BALANCE EQUATION

The similarity of form between Equations (10) and (35) should be emphasized at this point. This similarity is evident as well in the initial and boundary conditions. The initial condition, for example, is simply

$$T(0,z) = \hat{T}_I(z) \quad (37)$$

Flux-specified boundary conditions at the grid top and bottom are given respectively by

$$\left[-c^* \chi C_p D_H \left(\frac{\partial T}{\partial z} - \Gamma \right) \right] \Big|_{t,h} = \hat{q}_T(t) \quad (38)$$

$$\left[-c^* \chi C_p D_H \left(\frac{\partial T}{\partial z} - \Gamma \right) \right] \Big|_{t,0} = \hat{q}_B(t) \quad , \quad (39)$$

where $\hat{q}_T$ and $\hat{q}_B$ are specified heat fluxes (ergs/cm²·sec). As the relative velocity for temperature is that of the air, and we have specified that $w_A^i = 0$ at the boundaries, the inflow and outflow boundary conditions are not appropriate. We have, however, maintained the normal Dirichlet boundary condition.

These take the form

$$T(t,h) = \hat{T}_T(t) \quad (40)$$

and

$$T(t,0) = \hat{T}_B(t) \quad (41)$$

at the top and bottom boundaries.

E. OPERATOR SPLITTING

Equations (10) and (35) are *consolidated* forms, in the sense that they contain terms describing transport and generation. For the purposes of numerical approximation it is advantageous to segregate these terms by a so-called "splitting" process. For the mass-balance equation [Equation (10)], this yields:

$$\frac{\hat{D}c}{\hat{D}t} = \frac{\hat{D}c}{\hat{D}t} \Big|_{\text{transport}} + \frac{\hat{D}c}{\hat{D}t} \Big|_{\text{generation}} \quad (10')$$

where

$$\left. \frac{\hat{D}c}{\hat{D}t} \right|_{\text{transport}} = - \frac{\partial}{\partial z} \left[(w_r + w_A') c \right] + \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] + c \frac{\partial w_A'}{\partial z} + c \frac{w_A}{c^*} \frac{\partial c^*}{\partial z} \quad (42)$$

and

$$\left. \frac{\hat{D}c}{\hat{D}t} \right|_{\text{generation}} = G \quad (43)$$

A parallel form can be written for Equation (35):

$$\left. \frac{DT}{Dt} \right|_{\text{transport}} = - \frac{\partial}{\partial z} (w_A' T) + \frac{1}{c^* \chi} \frac{\partial}{\partial z} \left[c^* \chi D_H \frac{\partial T}{\partial z} \right] + T \frac{\partial w_A'}{\partial z} + w_A \Gamma - \frac{1}{c^* \chi} \frac{\partial}{\partial z} (c^* \chi D_H \Gamma) \quad (44)$$

and

$$\left. \frac{DT}{Dt} \right|_{\text{generation}} = \frac{\dot{H}^*}{c^* \chi C_p} \quad (45)$$

Equations (42) - (45) are applicable for the one-dimensional, time-dependent case. The corresponding equations for the two-dimensional, steady-state case are developed similarly from Equations (13) and (36); they are identical to the above equations except for a factor of $\left(\frac{u^*}{u_A} \right)$ on the right-hand side of each one.

3. CODE CHARACTERISTICS -- AN OVERVIEW

The objective of this section is to provide the reader with a fundamental exposure to the PLUVIUS, MOD 5.0 code, before the more detailed discussions of the example applications in the following sections. This preview can be segmented into the five separate areas of 1) initial rules and conventions, 2) logical flow, 3) data input, 4) modular construction, and 5) the zero-dimensional facility; these will be discussed individually in the following text. The successful user of PLUVIUS should have a moderate knowledge of the FORTRAN programming language. The text of this and the following sections is interspersed with many FORTRAN variable names and statements, which may be recognized by their appearance in upper-case.

A. INITIAL RULES AND CONVENTIONS

The computer code contains some important conventions, which are designed to maximize flexibility and computational efficiency. These conventions, which must be observed for successful code execution, are itemized in the following paragraphs.

- Dependent variables are stored in the two-dimensional array C. The array element C(I,K) is the value of the Kth variable or "species" at vertical grid point I. The index variables I and K are used consistently throughout PLUVIUS for vertical grid point and species. Two dependent variables that are not stored in the array C are air pressure and molar air density, which are held in the one-dimensional arrays PRESS and CS, respectively.
- Dependent variable values are temporarily held in the one-dimensional array CNN during the integration of the generation component of the mass balance equation at each grid point.
- The code contains two basic classes of dependent variables. The first is known as a "computed variable" and is calculated via the code's finite differencing procedure. The second is termed a "constrained variable." This class contains any variables that are not computed via the finite difference approximations, such as steady-state variables, variables

which do not change with time, and variables which are force-fit to observations. The ordering of dependent variables is set so that constrained variables follow computed variables. NCOMP is the number of computed variables and NCNSTR is the number of constrained variables, so that

$C(I,1) \dots C(I,NCOMP)$ are computed variables, and
 $C(I,NCOMP+1) \dots C(I,NCOMP+NCNSTR)$ are constrained variables.

It should be noted in this context that temperature, as well as pollutant and water species, can be treated as either a computed or constrained variable at the option of the user.

- Temperature and chemical species are identified within PLUVIUS, MOD 5.0 in the two following ways:
 - 1) by a numerical value of the species index (eg. $C(I,3)$ is the concentration at grid point I of the third species),
 - 2) by an associated species location variable, which must be defined by the user.

As an example, suppose that gaseous-phase SO_2 were designated as species number 3, such that the vector

$$C(I,3), \quad I = 1, \dots, N$$

defined the vertical column of SO_2 concentrations. By defining the species location variable

$$KS02G = 3$$

the equivalence

$$C(I,3) \equiv C(I,KS02G)$$

exists.

The above bookkeeping technique, while seemingly trivial at this point, is of large utility when dealing with complex multicomponent systems. Species location variables are held in the LOCATN common block and should be initialized in the SETUP subroutine, as described in the next section. Temperature must use the location variable KTEMP. The species which is

the sum of water vapor and cloud water must use the location variable KVAPCL when IFOG $\neq$ 0 (see following discussion of bypass variables). Other than this there is no restriction on the location variables, except that they be FORTRAN integers. The restriction in earlier versions of PLUVIUS that temperature be species 1 is not required in PLUVIUS, MOD 5.0.

- Turbulent diffusivities $D(I,L)$ are grouped to allow the versatility of having different diffusion coefficients for different classes of computed variables, if desired. The index L is known as the "diffusion regime." $L = 1$ always pertains to the diffusivity of heat in the energy equation regardless of whether or not this equation is actually used in the current computation. $L = 1$ cannot be used for any other species as it receives special treatment in the code appropriate only for temperature. The highest value of L (total number of separate diffusion regimes) is given by the variable LTD. Normally a minimum of two sets of diffusivities are required, one for heat and one for pollutant, corresponding to $LTD = 2$. The diffusion regime for each species is held in the array LDIF.

- Units employed consistently by the code are as follows:

material	gram-moles/cm ³
length	cm
temperature	°K
time	seconds
pressure	dynes/cm ²
energy	ergs

- Computations involving energy-balance calculations under saturated conditions (IFOG = 1) demand that one dependent variable be designated to describe the sum of cloud-water and water-vapor concentrations. As noted above, this variable is designated by the vector

$$C(I, KVAPCL) \quad I = 1, \dots, N.$$

B. LOGICAL FLOW

The primary logical flow in PLUVIUS, MOD 5.0 is demonstrated in the code's main program, as shown in Table C-1 in Appendix C. This program is

divided into three segments, as follows:

- Data input
- Initialization
- Major computation loop .

The data input segment reads values for a number of primary program variables, as described later in this section. In a specific application, the user might wish to add additional input. The appropriate location for this is in SETUP or other Class I subroutines, rather than the main program.

The initialization segment sets up the vertical grid spacing (via GRDSET), sets initial concentrations for dependent variables (via SETUP), and initializes various computational variables via calls to other subroutines. The running model-time variable, TCLOCK, is initialized to the input value of TSTART. During the initialization segment, the flag INIT has a value of 1, and several subroutines perform initialization code when INIT=1. Following initialization, the input data and initialized concentration arrays are printed, by executing the PRINT subroutine. The initialization flag INIT is then set equal to zero, and program flow proceeds to the major computation loop.

The major computation loop is executed repeatedly to integrate the mass- and energy-balance equations over the user specified time interval (TSTART to TSTOP). Each pass through the loop integrates the equations over a time step $2 \cdot DT$. As was noted in section 2-E, the transport and generation components of the governing equations have been "split." The basic $2 \cdot DT$ integration step has three parts:

- 1) integration of the transport component (Equations 42 and 44) for a time step DT , performed by subroutine ADVINT (see Table C-2),
- 2) integration of the generation component (Equations 43 and 45) for a time-step $2 \cdot DT$, performed by subroutine CHMINT (see Table C-3),
- 3) a second integration of the transport component for a time-step DT .

For each transport integration, the dependent variable values are stored in the array COLD, then four subroutines which provide transport parameters

are called (USHEAR, DIFF, VERT, SETTLE). During the first transport integration, subroutine TIMESP is called, which supplies a new value for the integration time step DT. This time step is determined primarily by numerical convergence criteria for the transport integration. Next, subroutine ADVINT is called, which performs the actual integration.

Following the ADVINT and CHMINT calls, results are printed and/or output to mass storage as appropriate. A check is made to determine whether the model's time limit (TSTOP) has been exceeded, and if not the major computation cycle is repeated. Upon successfully advancing beyond TSTOP, the code executes a normal Fortran stop.

C. DATA INPUT

Initial data are read in the main program by a simple sequence of READ statements, as shown in Table C-1. The first READ statement,

```
      READ (LUNIN,90000) MTITLE
90000  FORMAT (40A2)
```

reads a run title (up to 80 characters) which appears at the start of the model output.

The second READ statement,

```
      READ (LUNIN,90000) NCOMP, NCNSTR
90000  FORMAT (10I5)
```

identifies the number of species to be considered in the computation, as indicated previously:

NCOMP = number of species that will be modeled via finite-difference ("computed" approximation to Equations (10), (13), (35), or (36) and species) their appropriate boundary conditions.

NCNSTR = number of species, whose concentrations may vary with space ("constrained" and time, but are computed by methods that do not involve the species) finite-difference approximations.

The third READ statement,

```
      READ (LUNIN,90000) (NAME(LL,K), LL=1,5).
90000  FORMAT (40A2)
```

provides for input of alphanumeric variable names (e.g., OZONE, SO2). These alphanumeric names are for tabulated print-out only, and should not be confused with the "species location variables" described in Section 3A.

The fourth READ statement,

```
      READ (LUNIN,9020) N, LTD,DZ,GLEVL  
9020  FORMAT (2I5,2E10.3)
```

identifies the following variables:

N = number of grid points in vertical array,
LTD = total number of "diffusion regimes,"
DZ = the vertical grid spacing (when spacing is uniform),
GLEVL = elevation of grid bottom at computation's beginning.

The fifth READ statement,

```
      READ (LUNIN,9030) TSTART,TSTOP,DT  
9030  FORMAT (3E10.3)
```

informs the code of model start time, stop time, and initial time increment.

The sixth READ statement,

```
      READ (LUNIN,9040) NPRINT,DTPRIN,ITCOLL,DTCOLL  
140  FORMAT (I5,2E10.3)  
9040  FORMAT (I5,E10.3,I5,E10.3)
```

pertains to model output control. Model results may be printed either at regular model time intervals, or after a specified number of integration steps (which can have varying lengths). For regular time interval printout, set DTPRIN to the desired interval and NPRINT = 0. If NPRINT is positive (and DTPRIN = 0), then print-out will occur after each set of NPRINT time steps. ITCOLL and DTCOLL control model output to disk file as follows:

ITCOLL = 0 No disk file output.

ITCOLL = 1 Model output is time-averaged over intervals of DTCOLL, and then written to disk file.

ITCOLL = -1 Model output is written to disk file at intervals of DTCOLL, unaveraged.

The seventh READ statement,

```
      READ (LUNIN,90000) IGEN,IDIFF,ITEMP,IPRESS,ISETTL,IBOUND,IVERT,IFOG,  
      ISHEAR  
90000  FORMAT (10I5)
```

provides for bypassing of a number of subroutines, if their corresponding physical relationships are either constant in time or else unimportant to the modeling problem at hand. If the value of a bypass variable is set positive, its corresponding physical phenomenon is subjected to detailed, repetitive calculation and the appropriate subroutines are interrogated at each time step. If the variable is set equal to zero or a negative value, the related routines are either called only once, during initialization stage of the program execution, or else bypassed completely as appropriate. Significances of the bypass variables and their corresponding subroutines are listed in Table 3-1.

The bypass variable IFOG, which relates to water condensation, has the following effect. If IFOG is positive, then a species "water vapor and cloud vapor" must be used (KVAPCL, see above). The code checks whether the air is saturated or unsaturated at each grid point, and treats Equation (34) appropriately. If IFOG is zero or negative, then the code does not treat latent heat effects implicitly, and the dry form of the energy balance equation [Equation (27)] is used. In this case, the KVAPCL species need not be present. When ITEMP is non-positive, IFOG has no effect.

The eighth READ statement,

```
      READ (LUNIN,90500) ITOP(K), IBOT(K), LDIF(K), FILFAC(K)  
90500  FORMAT (3I5,E10.3)
```

specifies boundary-condition types, diffusion regimes, and filtering for each computed variable or species. ITOP and IBOT specify the types of boundary conditions at the top and bottom of the vertical grid, respectively. Setting these to positive values imposes flux-specified conditions. If they are set equal to zero, the boundary conditions become concentration-specified (inflow), and if they are negative the boundary conditions are treated as outflow conditions. LDIF specifies the diffusion regime for the species. FILFAC pertains to the smoothing filter, which is discussed at the very end of Appendix A. If FILFAC is set equal to zero, no filtering will be applied to the associated species.

TABLE 3-1: Significances of Bypass Control Variables

<u>Variable</u>	<u>Significance</u>	<u>Corresponding Subroutine</u>
IGEN	Physicochemical transformation	GEN and CHMINT
IDIFF	Atmospheric mixing	DIFF
ITEMP	Temperature	TEMPF
IPRESS	Pressure	PRESSF
ISSETTL	Terminal fall velocity	SETTL
IBOUND	Boundary conditions	BOUND
IVERT	Vertical air velocity	VERT
IFOG	Water condensation	No particular subroutine; bypasses at several locations throughout code
ISHEAR	vertical shear in horizontal wind field	USHEAR

The ninth READ statement,

```
      READ (LUNIN,9030) PRESS0,TEMP0  
9030  FORMAT (2E10.3)
```

inputs the pressure (dynes/cm²) and temperature (K) at grid position Z(1) at the initial stage of computation.

These nine READ statements complete the necessary input requirements for program execution. Examples of actual input and the corresponding computed output will be given in later sections of this report.

D. MODULAR CONSTRUCTION

As indicated in the previous text, the computer code is organized in a modular form, which is intended to provide the user with a large degree of versatility for specific applications. This subsection presents an overview of this structure by first discussing the modules on an individual basis, and then indicating how they operate as a composite whole. Examples of representative subroutines are given in the following sections.

Subroutines used by this code fall into three general classes:

1. Class I Subroutines - Those subroutines which are essential for basic operation of the code, and are intended for modular replacement by the user.
2. Class II Subroutines - Those subroutines which are essential for basic operation of the code and in general should be left unchanged by the user.
3. Class III Subroutines - Any additional subroutines, useful or necessary for a specific application, and supplied by the user. Often Class III subroutines are submodules of the major Class I subroutines.

Information exchange between the subroutines and the main program is conducted mainly with the use of blank and labeled COMMON. An example of these COMMON blocks, taken from the Example Application 1 of the next section,

is given in Table 3-2.^(a) The user will need to make the following modifications to these blocks for any particular application of PLUVIUS:

- 1) Set appropriate values for the parameters NZMAX, NCMAX, and NCTMAX. These parameters specify the maximum number of vertical grid points, "computed" variables, and "computed" + "constrained" variables, respectively, and must be set to accommodate the size of the application.
- 2) Specify appropriate species location variables in the LOCATN COMMON block.

The variable INIT, often appearing by itself in the subroutine argument list, is used as a flag to inform the subroutine whether initialization or "normal execution" is occurring. If INIT $\neq$ 1 the execution proceeds on the presumption that all initialization has been performed previously, with the result that several nonessential steps are bypassed. Setting of INIT to its appropriate value occurs automatically within the main program.

1. *Class I Subroutines*

To utilize PLUVIUS effectively, a user must have a good understanding of the Class I subroutines. It is through these Class I subroutines that the chemical, physical, and transport processes important to the user's application become part of the model. The ten Class I subroutines are summarized in Table 3-3, and are briefly described below. Examples of the routines provided in Sections 4 and 5 provide much additional information and insight about their usage.

SUBROUTINE ADJUST is applied to modify values of computed or constrained variables when these variables are limited by imposed constraints on the

(a)The reader will note that most of these COMMON blocks do not appear in the program and subroutine listings found in this manual. Rather, the statement "INCLUDE 'PLUVCMN'" is found near the start of most listings. This is an enhancement of standard FORTRAN-77 provided in many FORTRAN implementations. During compilation of a program unit, an INCLUDE statement is replaced by the lines of code in the named file (PLUVCMN in this case). Thus the INCLUDE statement is mainly a programming convenience which removes the need to reproduce lines of code in several places. Users not having an INCLUDE facility in their FORTRAN implementation will have to perform this code replacement themselves.

TABLE 3-2. Example Listing of PLUVIUS Common Blocks
(held in the PLUVCMN INCLUDE file)
for Example Application 1

```

PARAMETER ( NZMAX=21 )           ! NO. OF VERTICAL GRID POINTS
PARAMETER ( NCMAX=5 )           ! NO. OF "COMPUTED" VARIABLES
PARAMETER ( NCTMAX=10 )        ! NO. OF COMPUTED+CONSTRAINED VARIABLES

PARAMETER ( NNAMMX= NCTMAX+2 )
PARAMETER ( LUNIN=5, LUNOUT=6 )

COMMON /NAMES/ NAME(5,NNAMMX), MTITLE(40)

COMMON /PLUV/ COLD(NZMAX,NCTMAX), C(NZMAX,NCTMAX),
+   WR(NZMAX,NCMAX), WAP(NZMAX), WAGRID(NZMAX), D(NZMAX,4),
+   URATIO(NZMAX), LDIF(NCMAX), ITOP(NCMAX), IBOT(NCMAX),
+   FT(NCMAX), FB(NCMAX), CT(NCMAX), CB(NCMAX),
+   LTD, NCOMP, NCNSTR, NTOT, IGEN, IDIFF,
+   ITEMP, IPRESS, ISETTL, IBOUND, IVERT, IFOG, ISHEAR

COMMON /GRID/ N, NM1, DZ, DT, DTOLD, TCLOCK, TNEXT,
+   Z(NZMAX), GLEVL

COMMON / CHEM / CNN(NCTMAX), GGEN(NCTMAX), GDEC(NCTMAX),
+   CMIN(NCTMAX), DTSAVE(NZMAX)

COMMON/ODEINT/ NCORR, IEXP, EPS, DTMIN, RATESF(NCMAX),
+   CERROR(NCMAX)

COMMON /THERMO/ PRESS(NZMAX), CS(NZMAX), CPCSPS(NZMAX),
+   ISSAT(NZMAX), TEMP0, PRESS0

COMMON /LOCATN/ KTEMP,KA,KB,KC,KD,KE,KF,KG

COMMON / ADVDIF / ADIFFU(NZMAX,4), BDIFFU(NZMAX,4),
+   CDIFFU(NZMAX,4), DZDIZ(NZMAX), FTOLD(NCMAX), FBOLD(NCMAX),
+   WVAR(NZMAX), DWVCDI(NZMAX),
+   C1(NZMAX), C1DWAP(NZMAX), C1DLCS(NZMAX), D1ADV(NZMAX),
+   AMAT(2,2,NZMAX), BMAT(2,2,NZMAX), CMAT(2,2,NZMAX),
+   DVEC(2,NZMAX), UVEC(2,NZMAX)

```

TABLE 3-3. Summary of Class I Subroutines

Subroutine	Purpose
ADJUST	Modifies species values after advection integration step to meet imposed physical constraints.
BOUND	Sets boundary condition values for flux and concentration specified boundary conditions.
DIFF	Sets vertical eddy diffusivity coefficients.
GEN	Sets source and sink terms (physico-chemical generation and loss) for computed species. Also computes constrained species.
GRDSET	Sets vertical grid spacing.
SETTL	Sets settling velocity, w_r , for computed species.
SETUP	Sets initial values of computed and constrained variables.
TIMESP	Sets integration time step DT .
USHEAR	Sets horizontal air speed factor, u^*/u_A .
VERT	Sets the two components of the air vertical velocity, w_{A0} and w_A' .

system. ADJUST is applied after each advection integration step. The advection step may result in an "unphysical" relation between two closely linked species at a grid point, and an adjustment of these species is desirable. Also, some processes are more amenable to treatment by "adjustment" than by a rate law, such as nucleation scavenging of aerosols (see Section 5).

If there are no constraints of this type, then ADJUST should be supplied simply as a no operation stub. ADJUST does not have an associated bypass variable.

SUBROUTINE BOUND computes upper- and lower boundary conditions at each time step (if desired) for each of the computed species. If a boundary condition for species K is flux specified, then the appropriate flux value must be assigned to FB(K) and/or FT(K), where FB and FT are the vertical pollutant fluxes at the bottom and top boundaries. Fluxes are positive upwards and units are gram-moles/(cm² sec) [or ergs/(cm² sec) for temperature]. If a boundary condition is concentration-specified (inflow condition), then an appropriate concentration value is assigned to CB(K) (bottom boundary) or CT(K) (top). Outflow-specified boundary conditions are handled computationally and require no treatment in BOUND. If all boundary conditions do not vary with time, then the bypass variable IBOUND should be set to zero, and BOUND will be called only once, during initialization.

SUBROUTINE DIFF establishes the vector of vertical diffusion coefficients for each diffusion regime, D(I,L), I = 1,...,N, L = 1,...,LTD. Units are cm²/sec. Because of the finite-differencing procedure, D(I,L) is defined as the diffusivity between grid points I and I + 1. Remember that the diffusivity regime for temperature uses L = 1 and cannot be used for any other species. If diffusivities do not change with time, then repeated interrogations of this subroutine should be suppressed by setting IDIFF = 0.

SUBROUTINE GEN is used to specify chemical transformation and interphase transfer rates for each species, and is one of the most important Class I subroutines. These rates comprise the right-hand side of Equation (43), and are expressed as

$$G_K = GGEN(K) - GDEC(K)$$

where GGEN(K) is the generation rate (source terms) and GDEC is the decay rate (sink terms) for species K. For situations in which temperature is treated as a computed variable,

$$\frac{\dot{H}^*}{c^* \chi C_p} = \text{GGEN}(\text{KTEMP}) - \text{GDEC}(\text{KTEMP})$$

as indicated in Equation (47). [Note that $c^* \chi C_p$ is computed in SUBROUTINE TEMPF and stored in the array CPCSPS(I), $I = 1, \dots, N$].

Segregation of G into generation and decay terms is necessary because of requirements of the calling routine, ODEINT, which performs numerical integrations of the rate terms. It should be noted, however, that such segregation is mandatory only for stiff mathematical systems. If the species of interest reacts only slowly and does not approach equilibrium, then it is permissible to set GDEK = 0, and consolidate both sources and sink terms into GGEN. Further discussion of this stiffness property and the ODEINT integrator are given in Appendix B.

GEN is also used for calculating constrained variables. These include variables that are computed on the basis of equilibrium assumptions, as well as those determined in a variety of possible alternative ways. These computations are performed in GEN because for many systems, the calculation of equilibrium or steady-state species is often intertwined with the calculation of rates of change for nonequilibrium species.

A minor inefficiency results from this organization because constrained species must be recomputed before output occurs. Thus the flag IGCALC is provided in calls to GEN. When IGCALC is positive, both constrained variables and generation and decay rates must be calculated. When IGCALC is zero, only constrained variables are needed. Some improvement in efficiency will result if the two calculations can be segregated, but the user should not try to force this segregation if it is unnatural for the problem at hand.

GEN is different from the other Class I subroutines in that GEN is called separately for each vertical grid point. The vertical index, I, is passed to

GEN as a subroutine parameter. GEN uses the one-dimensional array CNN to hold current values of the dependent variables.

If the bypass variable IGEN is set nonpositive, then GEN is not called at all, and the integration of the generation component (Equation 43 and 45) is skipped.

SUBROUTINE GRDSET establishes the vertical finite-difference grid by assigning values to the grid-height array, Z(I). Grid spacing may be uniform [$Z(I) - Z(I-1) = \text{constant}$], or nonuniform, at the user's preference. For a uniform grid, the input variable DZ can be used to specify the grid spacing [$Z(I) = (I-1)*DZ$]. GRDSET is called only once, during initialization, and the grid spacing remains fixed during a model run.

SUBROUTINE SETTLE computes settling velocities, w_r , as defined in Equation (4). Settling velocities for each species (K) at each grid location (I) are assigned to array elements WR(I,K). Units are cm/sec, and downward velocities are negative. Many species (gases, submicron aerosols, temperature) will have zero or negligible settling velocities, whereas precipitation-borne species will have significant fall velocities. If the bypass variable ISETTL is set nonpositive, then SETTLE is called only once, during initialization.

SUBROUTINE SETUP sets the initial values of computed and constrained variables. Constrained variables may be set directly, or by calling GEN. After the initial temperature values are set, a call to PRESSF should be made to set pressure and air density. Other important tasks performed by SETUP are assigning values to species location variables, and initializing several parameters used by the ODEINT integrator. SETUP is called only once by PLUVIUS, during initialization.

SUBROUTINE TIMESP defines the basic integration time step, DT, for the next pass through the major computation loop. DT is completely variable from one time step to the next. It can be set to a constant value throughout the computation, or it may be adjusted to meet user demands. From an efficiency standpoint, it is desirable that DT be large. When vertical advection is significant, then computational constraints place limits on DT (see Example Application 2).

SUBROUTINE USHEAR is necessary for two-dimensional, steady-state simulations involving wind shear. The subroutine sets the vector

$$\text{URATIO}(I) = \frac{u^*}{u_A/z(I)}, \quad I = 1, \dots, N$$

where the ratio on the right hand side is from Equation (13) and (36). For simulations with no shear (which includes all one-dimensional time-dependent simulations), URATIO should be set equal to 1. When the bypass variable ISHEAR is set non-positive, USHEAR is called only once, during initialization.

SUBROUTINE VERT is used to set the vertical air velocity, w_A . In computations involving cloud and precipitation formation, w_A is a very important parameter since the rate of moisture condensation is directly proportional to it. As indicated in Equations (8) and (11), the vertical air velocity is partitioned into two sub-components: the "grid vertical velocity", which is the rate of change of the vertical position of the computational grid, and the "relative vertical air velocity", which is the velocity of upward airflow through the computational grid. VERT simply assigns the grid vertical velocity values to the vector WAGRID(I), and the relative vertical air velocity values to the vector WAP(I). Units are cm/sec.

For one-dimensional time-dependent simulations [Equation (8)], the grid vertical velocity is given by w_{A0} and is thus constant with height. For the two-dimensional, steady-state simulations with horizontal wind shear, the vertical grid velocity is given by $w_{A0} \cdot (u_A/u_{A0})$ [Equation (11)], and will vary with height. Using the variable URATIO, which is set in SUBROUTINE USHEAR, we can write

$\text{WAGRID}(I) \equiv$ vertical grid velocity at grid I

$$\begin{aligned} &\equiv w_{A0} \left(\frac{u_A}{u_{A0}} \right) = w_{A0} \left(\frac{u^*}{u_{A0}} \right) / \left(\frac{u^*}{u_A} \right) \\ &= \text{WAGRID}(1) * \text{URATIO}(1) / \text{URATIO}(I) \end{aligned}$$

Note that w_{A0} is defined as the grid vertical velocity at the surface (bottom grid). VERT also has a bypass variable, IVERT, which, when set non-positive, causes VERT to be called only once, during initialization.

2. *Class II Subroutines*

As noted previously, Class II subroutines are not normally intended for user modification (modify at your own risk!), and thus will not be discussed in detail here. The subroutines group naturally into three subclasses: computational routines involved in the numerical integrations, thermodynamic routines, and output routines. The names and purposes of these subroutines are summarized in Table 3-4 for overview purposes. Complete listings of all Class II subroutines are presented in Appendix C, along with a description of many of the variables used throughout the code. The user may wish to tailor the two output routines to his specific needs, and this can generally be done without fear of side effects on the rest of the code.

E. "ZERO-DIMENSIONAL" TESTING FACILITY

When working with complex physicochemical systems, it is desirable to test the generation component of the model (SUBROUTINE GEN) with only 1 or 2 grid points, rather than 20 or 30, simply to reduce computer usage. With a grid of this size (1 or 2), the advection and diffusion terms become meaningless. In PLUVIUS MOD 5.0, there is a facility which essentially bypasses the transport integration when the number of vertical grid points, N, is specified as 1 or 2 in the input data. Thus the user may switch back and forth between complete runs and generation component tests, simply by changing N in the input data.

In actuality, SUBROUTINE ADVINT is not completely bypassed. However, when N is 1 or 2, ADVINT skips its normally executed code and instead calls SUBROUTINE ZERODM. ZERODM simulates those physical effects that result if the grid is moving vertically with grid velocity WAGRID(1). If the grid is rising, then 1) pollutant concentrations decrease slowly because the air is expanding, and 2) the temperature cools adiabatically (if it is a "computed"

TABLE 3-4. Summary of Class II Subroutines

<u>Sub-Class</u>	<u>Subroutine</u>	<u>Purpose</u>
Computa- tional	ADVINT	Performs numerical integration of the advection-diffusion component of the governing equations.
	CHMINT	Controls the numerical integration of the generation component of the governing equations. (Actual integration performed by ODEINT.)
	DERIV	Provides species independent coefficients for the mass balance equation to ADVINT.
	FILTER	Applies nonlinear filter after each advection-diffusion integration step to reduce "short-wave noise" (see Appendix A).
	FIRSTD	Calculates the first vertical derivative of a vector.
	ODEINT	Performs actual numerical integration of the generation component of the governing equations (called by CHMINT).
	SETVEC	Provides species dependent coefficients for the mass balance equation to ADVINT.
	TEMPF	Provides coefficients for the energy balance equation to ADVINT.
	TRIDG2	Solves simultaneous linear equations with tridiagonal coefficient matrix, when unknowns are two-element vectors.
	TRIDAG	Solves simultaneous linear equations with tridiagonal coefficient matrix, when unknowns are scalars.
Thermo- dynamic	ZERODM	Computes affects of vertical motions for "zero-dimensional" mode.
	PRESSF	Computes pressure by integrating the hydrostatic equation and sets air densities.
	RHOAIR	Function returns air density for specified temperature and pressure.

TABLE 3-4 Continued

<u>Sub-Class</u>	<u>Subroutine</u>	<u>Purpose</u>
Output	RLAPSE	Function returns dry or moist adiabatic lapse rate for specified temperature and air density.
	SAT	Function returns saturation vapor concentration over water for specified temperature.
	COLLECT	Writes model results to mass storage for later plotting, etc.
	PRINT	Writes model results to line printer.

variable). If WAGRID(1) is set to zero, then ZERO DM has no effect whatever, and only the generation component of the code is exercised. The ability to specify a non-zero vertical velocity can be useful when the simulation includes cloud formation processes.

4. EXAMPLE APPLICATION 1: SIMPLE AIR CHEMISTRY AND DRY DEPOSITION

This section describes a very simplistic application of the PLUVIUS code. The purpose of this application is to provide an uncomplicated example of the use of the Class I subroutines and the input to and output from a PLUVIUS run. Because of this the physics and chemistry in the example have been purposely kept to a minimum.

The example simulates the evolution of a line-source plume. The plume is held in a 1-km-deep boundary layer which is capped by an impervious inversion, and the line source is at a height of 0.5 km. The plume is advected downwind from the source by a horizontal wind which is constant in height, so the example is treated as one-dimensional, time-dependent. The simulation begins at a position corresponding to a travel time of 500 seconds from the source, and runs for an additional 3000 seconds.

There are eight dependent variables in the example: seven hypothetical species, labeled "A" through "G", and temperature. The physical and chemical properties of these variables are summarized in Table 4-1. Species A, B, C, and D are "source" species in the plume. Species A and B are chemically inert, while C and D react to form the product species E. Species F represents a constrained "background" variable which has a constant mixing ratio. Species G is a constrained variable which is in equilibrium with C and F. Temperature is treated as a constrained variable in this example, following a dry adiabatic lapse rate.

A. INPUT DATA

Input data for this example are given in Table 4-2, and they should be compared with the input statements described in Section 3. The first input line is a run title which will appear on the printed output. The second input line specifies that there are five computed variables and three

TABLE 4-1. Summary of Properties of Species in Example Application 1

Species	Computed/ Constrained	Chemical Reaction	Surface Deposition	Settling	Initial Concentration
A	Computed	none	none	none	Gaussian ^(a)
B	Computed	none	$v_d = 1$ cm/sec ^(b)	none	Gaussian
C	Computed	$C + D \xrightarrow{k} E$ with $k = 10^7$ cm ³ /mole·sec $C + F \xrightleftharpoons[k_r]{k_f} G$ with $k_f/k_r = 1$ cm ³ /mole	none	none	Gaussian
D	Computed	$C + D \rightarrow E$	surface acts as total sink	none	Gaussian
E	Computed	$C + D \rightarrow E$	$v_d = 2$ cm/sec	$w_r = 1$ cm/sec	zero
F	Constrained to 10^{-7} mixing ratio				
G	Constrained to equilibrium with C and F by $C + F \rightleftharpoons G$				
Temp	Constrained to dry adiabatic profile, 288 K at surface				

(a) Gaussian - see discussion in text.

(b) v_d is deposition velocity.

TABLE 4-2. Input Data For Example 1.

<u>Line</u>	<u>Data</u>
1:	EXAMPLE RUN 1 - PLUVIUS MOD 5.0 USER MANUAL
2:	5 3
3:	A
4:	B
5:	C
6:	D
7:	E
8:	F
9:	G
10:	TEMP
11:	21 2 5.0E3 0.0
12:	0.5E3 3.5E3 1.0E2
13:	10 0.0 -1 3.0E3
14:	1 0 0 0 0 1 0 0 0
15:	1 1 2 0.0
16:	1 1 2 0.0
17:	1 1 2 0.0
18:	1 0 2 0.0
19:	1 1 2 0.0
20:	1.016E6 288.6

constrained variables in the example. The next eight input lines provide names for each variable, for use during program output.

Input line 11 specifies that the vertical grid consists of 21 grid points, that there are two "diffusion regimes", that the uniform grid spacing is 5000 cm, and that the initial height of the bottom grid point (GLEVL) is at 0 cm. Input line 12 specifies that the simulation begins at a time of 500 seconds, terminates at a time of 3500 seconds, and uses an initial integration time step of 100 seconds. Input line 13 specifies output control information. As NPRINT is specified positive (5), printed output will occur after every fifth integration cycle (remember that an integration cycle involves two advection-diffusion time steps). As ITCOLL is specified to be zero, no output to disk file will be made.

Input line 14 specifies the bypass variables. Only IGEN and IBOUND are positive, so only the CLASS I subroutines GEN and BOUND will be interrogated regularly. For this example, the information that is provided by the other CLASS I subroutines does not change with time, so the subroutines only need to be interrogated once at the start of the program.

Input lines 15 through 19 specify the boundary conditions, diffusion regimes, and filter factors for each of the five computed species. Each species uses diffusion regime 2 (remember that regime 1 is reserved for temperature). No filtering is applied (FILFAC = 0.). All the species besides D have flux-specified boundary conditions at both the top and bottom boundaries. Species D has a concentration-specified bottom boundary condition. The final input line specifies initial surface pressure and temperatures of $1.016 \cdot 10^6$ dynes/cm² and 288.6K.

B. CLASS I SUBROUTINE DESCRIPTIONS

As discussed in Section 3, the ten Class I subroutines are the primary mechanism by which the physics and chemistry appropriate to a particular application are inserted into the PLUVIUS framework. Thus it is extremely important that the user have a good understanding of the function of each. The listings and discussions of these subroutines for our simple example

which are given below should serve to clarify the initial subroutine descriptions of Section 3.

SUBROUTINE SETUP (Table 4-3)

SETUP defines the initial concentration profiles for the dependent variables and state variables, and also defines the species location variables.

The species location variables are defined in the initial data statements; e.g., the variable KA is used as a location index for species A and has a value 1. Note that these values must correspond exactly to the ordering of species given in the input data (e.g., A is first, and TEMP is last). The next data statements initialize parameters used by ODEINT.

The first executable statements compute the initial temperature profile, which follows a dry adiabatic lapse rate. Next, subroutine PRESSF is called which computes the initial pressure and air density fields. Note that air density is used to initialize some of the other species in terms of mixing ratio, so the thermodynamic variables are computed first.

Next, the species A through G are initialized. The four "Gaussian" species are initialized so that their mixing ratios follow a Gaussian distribution, peaked at 0.5 km with a peak mixing ratio value of 10^{-6} . The initial vertical plume-spread parameter, SIGMAZ, is 10^4 cm and was chosen to correspond to 500 seconds of travel time from a line source at a specified diffusivity of 10^5 cm²/sec. Species E is initialized to a zero concentration.

SUBROUTINE ADJUST (Table 4-4)

In this simple example, no "adjustment" is required. Thus the subroutine is provided as a do-nothing "stub."

SUBROUTINE BOUND (Table 4-5)

BOUND provides values for flux or concentration specified boundary conditions. For this example, the top boundary is an impervious inversion, so the flux at the top boundary (FT) is set to zero for each of the computed species. Species A and C are non-depositing (see Table 4-1), so their fluxes at the bottom boundary (FB) are also zero.

TABLE 4-3. Listing of Subroutine SETUP for Example Application 1

```

SUBROUTINE SETUP

  INCLUDE 'PLUVCMN'

C
C  ESTABLISH SPECIES INDEX NAMES AND CONVERSION FACTORS
C
  DATA KA, KB, KC, KD, KE, KF, KG /1,2,3,4,5,6,7/
  DATA KTEMP/8/

C
C  ESTABLISH PARAMETERS USED IN O.D.E. INTEGRATION ROUTINE (ODEINT)
C
  DATA EPS/1.E-2/, DTMIN/1.E-15/, RATESF/NCMAX*1.E-2/
  DATA NCORR/1/, IEXP/0/
  DATA CMIN/NCTMAX*1.E-25/
  DATA CERROR/NCMAX*1.E-21/

C
C  ESTABLISH INITIAL TEMPERATURE AS DRY ADIABATIC, THEN CALL
C  PRESSF TO COMPUTE PRESSURE AND AIR DENSITY
C
  C(1,KTEMP) = TEMP0
  TMPDUM = TEMP0
  DO I = 2, N
    TMPDUM = TMPDUM - 9.76E-5*(Z(I)-Z(I-1))
    C(I,KTEMP) = TMPDUM
  END DO
  CALL PRESSF(1)

C
C  SET INITIAL VALUES OF SPECIES CONCENTRATIONS FOR COMPUTED SPECIES
C
  DO I = 1, N
    C(I,KA) = 1.E-6*CS(I)*EXP(-(Z(I)-50000.0)**2/2.E8)
    C(I,KB) = C(I,KA)
    C(I,KC) = C(I,KA)
    C(I,KD) = C(I,KA)
    C(I,KE) = 0.
  END DO

  RETURN
END

```


TABLE 4-4. Listing of Subroutine ADJUST for Example Application 1

```
SUBROUTINE ADJUST
RETURN
END
```

TABLE 4-5. Listing of Subroutine BOUND for Example Application 1

```
SUBROUTINE BOUND( INIT )
INCLUDE 'PLUVCMN'

DO K = 1, NCOMP
    FT(K) = 0.
    FB(K) = 0.
END DO
CB(KD) = 0.

FB(KB) = -1.*C(1,KB)
FB(KE) = -2.*C(1,KE)

RETURN
END
```

TABLE 4-6. Listing of Subroutine DIFF for Example Application 1

```
SUBROUTINE DIFF(INIT)
INCLUDE 'PLUVCMN'

DO I = 1, N
    D(I,2) = 1000000.
END DO

RETURN
END
```

Species B and E dry deposit with deposition velocities of 1 and 2 cm/sec, respectively. For these species, the bottom flux is just the product of the current concentration and the deposition velocity (with negative sign). For species D, the surface acts as a total sink, so its concentration is always zero at the bottom boundary. This is accomplished by setting CB(KD) equal to zero.

SUBROUTINE DIFF (Table 4-6)

DIFF sets the vertical eddy diffusivities for each diffusion regime. In this example, two diffusion regimes are required, but regime 1 is never used, since it is reserved for temperature and temperature is a constrained variable in this case. For regime 2, a constant eddy diffusivity of $10^5 \text{ cm}^2/\text{sec}$ is used. Because the diffusivity is constant in time, the bypass variable IDIFF can be set to zero.

SUBROUTINE GEN (Table 4-7)

GEN computes generation and decay rates for the computed species, and also sets constrained species. The first part of the example routine sets the values for species F and G. The reader may wonder why temperature is not set here also, since it too is a constrained species. For this example, temperature is constant in time, and was already initialized in SETUP. Thus there is no computational need to reset its value in GEN. Constrained species whose concentrations change with time should be set in GEN, but those that are constant in time may be established in SETUP, at the user's preference.

The second portion of GEN computes generation and decay rates. Of the two reactions shown in Table 4-1, only the first, which involves C, D, and E, need be treated here. The others simulate an equilibrium situation, and so produce no net gain or loss. Note that GEN works with the CNN array, rather than the C array.

SUBROUTINE GRDSET (Table 4-8)

GRDSET establishes the vertical spacing of the computational grid. For this example, a uniform spacing is used, so the code is trivial. For uniform spacing, the input variable DZ can be used to read in the grid spacing.

TABLE 4-7. Listing of Subroutine GEN for Example Application 1

```
SUBROUTINE GEN( I, IGCALC, TGEN, DTAU, JPASSO )
INCLUDE 'PLUVCMN'
```

C
C
C

```
SET CONSTRAINED VARIABLES
```

```
CNN(KF) = 1.E-7*CS(I)
CNN(KG) = CNN(KF)*CNN(KC)
IF (IGCALC .EQ. 0) RETURN
```

C
C
C

```
SET GENERATION AND DECAY RATES
```

```
DO K = 1, NCOMP
    GGEN(K) = 0.
    GDEC(K) = 0.
END DO

GDEC(KC) = CNN(KC)*CNN(KD)*1.E7
GDEC(KD) = GDEC(KC)
GGEN(KE) = GDEC(KC)
```

```
RETURN
END
```

TABLE 4-8. Listing of Subroutine GRDSET for Example Application 1

```
SUBROUTINE GRDSET
INCLUDE 'PLUVCMN'
```

```
Z(1) = 0.
DO I = 2, N
    Z(I) = Z(I-1) + DZ
END DO
```

```
RETURN
END
```

SUBROUTINE SETTLE (Table 4-9)

SETTLE establishes the settling velocities of the computed variables. For this example, only species E has a settling velocity, 1 cm/sec. This velocity is constant with time, so the bypass variable ISETTLE can be set to zero.

SUBROUTINE TIMESP (Table 4-10)

TIMESP sets the basic integration time step, DT. In this example, there are no serious computational limitations, and a fixed time step of 100 seconds is used. A fixed time step can be established when the initial value of DT is read in as part of the input, so TIMESP does nothing in this example.

SUBROUTINE USHEAR (Table 4-11)

USHEAR establishes the ratio $URATIO = u^*/u_A$. For one-dimensional, time-dependant simulations, this ratio is always unity.

SUBROUTINE VERT (Table 4-12)

VERT establishes the two components of the air vertical velocity. In this example, the air vertical velocity is zero throughout the simulation, so the code is trivial.

C. EXAMPLE OUTPUT

Some of the output for this example application is shown in Tables 4-13 to 4-15. Table 4-13 shows a heading page which is produced at the start of each run. The page summarizes the dependent variables and other control data provided as input.

Table 4-14 shows the initial species concentrations at the start of the simulation, at time TCLOCK = 500 seconds. Each column in the table shows a particular dependent variable. Pressure ("P") and air density ("CS") are also listed. Each row corresponds to a different vertical grid point. Heights are shown in kilometers to improve readability, although centimeters are used internally in the program. The four "Gaussian" species, A through D, have identical initial concentration profiles which maximize at 0.5 km above ground level. These distributions are slightly skewed with height

TABLE 4-9. Listing of Subroutine SETTLE for Example Application 1

```

SUBROUTINE SETTLE(INIT)
  INCLUDE 'PLUVCNM'

  DO I = 1, N
    DO K = 1, NCOMP
      WR(I,K) = 0.
    END DO
    WR(I,KE) = -1.
  END DO

  RETURN
END

```

TABLE 4-10. Listing of Subroutine TIMESP for Example Application 1

```

SUBROUTINE TIMESP
  INCLUDE 'PLUVCNM'
  DT = 100.
  RETURN
END

```

TABLE 4-11. Listing of Subroutine USHEAR for Example Application 1

```

SUBROUTINE USHEAR(INIT)
C
C  USHEAR SETS URATIO(I) = UA(IREF)/UA(I) WHERE
C    UA = THE HORIZONTAL WIND SPEED AT HEIGHT Z(I)
C    IREF = A SPECIFIED REFERENCE LEVEL (FIXED FOR THE MODEL RUN)
C  FOR ONE-DIMENSIONAL TIME-DEPENDENT SIMULATIONS WITH NO SHEAR,
C    SET URATIO(I) = 1. FOR ALL I.
C
  INCLUDE 'PLUVCNM'

  DO I = 1, N
    URATIO(I) = 1.
  END DO

  RETURN
END

```

TABLE 4-12. Listing of Subroutine VERT for Example Application 1

```

SUBROUTINE VERT
  INCLUDE 'PLUVCMN'
C
C   VERT SETS THE VERTICAL AIR-VELOCITY COMPONENTS
C   WAGRID - VERTICAL VELOCITY OF GRID
C   WAP - VERTICAL AIR VELOCITY RELATIVE TO GRID
C
C   NOTE: FOR CALCULATIONS INVOLVING SHEAR (URATIO NOT CONSTANT),
C   THEN (WAGRID*URATIO) MUST BE CONSTANT. UNDER SUCH CONDITIONS,
C   SET WAP SO THAT (WAP + WAGRID) EQUALS THE TOTAL WA.
C   (I.E., WAGRID AND WAP JUST PARTITION THE TOTAL VERTICAL VELOCITY).
C
  DO I = 1, N
    WAP(I) = 0.
    WAGRID(I) = 0.
  END DO

  RETURN
END
```

TABLE 4-13. Output Heading Page From Example Application 1

```

+++++
+
+   PLUVIUS   REACTIVE   STORM   MODEL   (MOD 5.0)   +
+
+++++

```

RUN ID: EXAMPLE RUN 1 - PLUVIUS MOD 5.0 USER MANUAL

COMPUTED SPECIES		TOP B.C.	BOTTOM B.C.	DIFFUS. REGIME	FILTER FACT.
1	A	FLUX	FLUX	2	0.00
2	B	FLUX	FLUX	2	0.00
3	C	FLUX	FLUX	2	0.00
4	D	FLUX	CONC.	2	0.00
5	E	FLUX	FLUX	2	0.00

CONSTRAINED SPECIES

6	F
7	G
8	TEMP

CONTROL DATA

IGEN	1	IPRESS	0	IVERT	0
IDIFF	0	ISETTL	0	IFOG	0
ITEMP	0	IBOUND	1	ISHEAR	0

TSTART	500.0	(0.14 HRS)	NPRINT	0
TSTOP	3500.0	(0.97 HRS)	DTPRIN	1000.0
			DTCOLL	0.0

UNITS USED IN PLUVIUS ARE CGS:

TIME	SEC
HEIGHT	CM
VELOCITY	CM/SEC
TEMPERATURE	DEG K
MASS	GM
PRESSURE	DYNES/CM**2
ENERGY	ERGS
CONCENTRATION	GM MOLE/CM**3

(NOTE: THIS IS CONCENTRATION PER VOLUME OF TOTAL SPACE (AIR),
NOT CONCENTRATION PER VOLUME OF LIQUID)

ALL OUTPUT IN THESE UNITS UNLESS OTHERWISE NOTED

TABLE 4-14. Model Output at TCLOCK = 500 Seconds From Example Application 1

TCLOCK	500.00	(0.139 HRS)			GLEVL (KM)		0.000			
DT	100.00				WAGRID(1)		0.00			
Z (KM)	A	B	C	D	E	F	G	TEMP	P	CS
1.000	0.1448E-15	0.1448E-15	0.1448E-15	0.1448E-15	0.1000E-24	0.3885E-11	0.5625E-27	0.2788E+03	0.9007E+06	0.3885E-04
0.950	0.1563E-14	0.1563E-14	0.1563E-14	0.1563E-14	0.1000E-24	0.3902E-11	0.6101E-26	0.2793E+03	0.9063E+06	0.3902E-04
0.900	0.1315E-13	0.1315E-13	0.1315E-13	0.1315E-13	0.1000E-24	0.3919E-11	0.5153E-25	0.2798E+03	0.9118E+06	0.3919E-04
0.850	0.8611E-13	0.8611E-13	0.8611E-13	0.8611E-13	0.1000E-24	0.3936E-11	0.3390E-24	0.2803E+03	0.9174E+06	0.3936E-04
0.800	0.4392E-12	0.4392E-12	0.4392E-12	0.4392E-12	0.1000E-24	0.3954E-11	0.1736E-23	0.2808E+03	0.9230E+06	0.3954E-04
0.750	0.1745E-11	0.1745E-11	0.1745E-11	0.1745E-11	0.1000E-24	0.3971E-11	0.6927E-23	0.2813E+03	0.9286E+06	0.3971E-04
0.700	0.5397E-11	0.5397E-11	0.5397E-11	0.5397E-11	0.1000E-24	0.3988E-11	0.2152E-22	0.2818E+03	0.9343E+06	0.3988E-04
0.650	0.1300E-10	0.1300E-10	0.1300E-10	0.1300E-10	0.1000E-24	0.4005E-11	0.5208E-22	0.2823E+03	0.9400E+06	0.4005E-04
0.600	0.2440E-10	0.2440E-10	0.2440E-10	0.2440E-10	0.1000E-24	0.4023E-11	0.9815E-22	0.2827E+03	0.9457E+06	0.4023E-04
0.550	0.3565E-10	0.3565E-10	0.3565E-10	0.3565E-10	0.1000E-24	0.4040E-11	0.1440E-21	0.2832E+03	0.9514E+06	0.4040E-04
0.500	0.4057E-10	0.4057E-10	0.4057E-10	0.4057E-10	0.1000E-24	0.4057E-11	0.1646E-21	0.2837E+03	0.9571E+06	0.4057E-04
0.450	0.3596E-10	0.3596E-10	0.3596E-10	0.3596E-10	0.1000E-24	0.4075E-11	0.1465E-21	0.2842E+03	0.9629E+06	0.4075E-04
0.400	0.2482E-10	0.2482E-10	0.2482E-10	0.2482E-10	0.1000E-24	0.4092E-11	0.1016E-21	0.2847E+03	0.9687E+06	0.4092E-04
0.350	0.1334E-10	0.1334E-10	0.1334E-10	0.1334E-10	0.1000E-24	0.4110E-11	0.5484E-22	0.2852E+03	0.9745E+06	0.4110E-04
0.300	0.5586E-11	0.5586E-11	0.5586E-11	0.5586E-11	0.1000E-24	0.4128E-11	0.2306E-22	0.2857E+03	0.9804E+06	0.4128E-04
0.250	0.1821E-11	0.1821E-11	0.1821E-11	0.1821E-11	0.1000E-24	0.4145E-11	0.7550E-23	0.2862E+03	0.9863E+06	0.4145E-04
0.200	0.4625E-12	0.4625E-12	0.4625E-12	0.4625E-12	0.1000E-24	0.4163E-11	0.1925E-23	0.2866E+03	0.9922E+06	0.4163E-04
0.150	0.9145E-13	0.9145E-13	0.9145E-13	0.9145E-13	0.1000E-24	0.4181E-11	0.3823E-24	0.2871E+03	0.9981E+06	0.4181E-04
0.100	0.1408E-13	0.1408E-13	0.1408E-13	0.1408E-13	0.1000E-24	0.4198E-11	0.5913E-25	0.2876E+03	0.1004E+07	0.4198E-04
0.050	0.1689E-14	0.1689E-14	0.1689E-14	0.1689E-14	0.1000E-24	0.4216E-11	0.7122E-26	0.2881E+03	0.1010E+07	0.4216E-04
0.000	0.1578E-15	0.1578E-15	0.1578E-15	0.1578E-15	0.1000E-24	0.4234E-11	0.6681E-27	0.2886E+03	0.1016E+07	0.4234E-04

TABLE 4-15. Model Output at TCLOCK = 3500 Seconds From Example Application 1

TCLOCK	3500.00	(0.972 HRS)			GLEVL (KM)		0.000			
DT	100.00				WAGRID(1)		0.00			
Z (KM)	A	B	C	D	E	F	G	TEMP	P	CS
1.000	0.4957E-11	0.4957E-11	0.3821E-11	0.3821E-11	0.9145E-12	0.3885E-11	0.1484E-22	0.2788E+03	0.9007E+06	0.3885E-04
0.950	0.5206E-11	0.5206E-11	0.3982E-11	0.3982E-11	0.1027E-11	0.3902E-11	0.1554E-22	0.2793E+03	0.9063E+06	0.3902E-04
0.900	0.5897E-11	0.5897E-11	0.4421E-11	0.4421E-11	0.1276E-11	0.3919E-11	0.1733E-22	0.2798E+03	0.9118E+06	0.3919E-04
0.850	0.6981E-11	0.6981E-11	0.5095E-11	0.5095E-11	0.1666E-11	0.3936E-11	0.2006E-22	0.2803E+03	0.9174E+06	0.3936E-04
0.800	0.8371E-11	0.8371E-11	0.5943E-11	0.5943E-11	0.2187E-11	0.3954E-11	0.2350E-22	0.2808E+03	0.9230E+06	0.3954E-04
0.750	0.9950E-11	0.9950E-11	0.6882E-11	0.6881E-11	0.2813E-11	0.3971E-11	0.2732E-22	0.2813E+03	0.9286E+06	0.3971E-04
0.700	0.1157E-10	0.1157E-10	0.7821E-11	0.7819E-11	0.3497E-11	0.3988E-11	0.3119E-22	0.2818E+03	0.9343E+06	0.3988E-04
0.650	0.1307E-10	0.1307E-10	0.8670E-11	0.8667E-11	0.4176E-11	0.4005E-11	0.3473E-22	0.2823E+03	0.9400E+06	0.4005E-04
0.600	0.1430E-10	0.1430E-10	0.9349E-11	0.9343E-11	0.4772E-11	0.4023E-11	0.3761E-22	0.2827E+03	0.9457E+06	0.4023E-04
0.550	0.1511E-10	0.1511E-10	0.9793E-11	0.9780E-11	0.5212E-11	0.4040E-11	0.3956E-22	0.2832E+03	0.9514E+06	0.4040E-04
0.500	0.1542E-10	0.1542E-10	0.9961E-11	0.9935E-11	0.5437E-11	0.4057E-11	0.4042E-22	0.2837E+03	0.9571E+06	0.4057E-04
0.450	0.1519E-10	0.1519E-10	0.9838E-11	0.9788E-11	0.5415E-11	0.4075E-11	0.4009E-22	0.2842E+03	0.9629E+06	0.4075E-04
0.400	0.1444E-10	0.1444E-10	0.9436E-11	0.9342E-11	0.5151E-11	0.4092E-11	0.3862E-22	0.2847E+03	0.9687E+06	0.4092E-04
0.350	0.1327E-10	0.1326E-10	0.8795E-11	0.8626E-11	0.4681E-11	0.4110E-11	0.3615E-22	0.2852E+03	0.9745E+06	0.4110E-04
0.300	0.1181E-10	0.1178E-10	0.7978E-11	0.7683E-11	0.4069E-11	0.4128E-11	0.3293E-22	0.2857E+03	0.9804E+06	0.4128E-04
0.250	0.1020E-10	0.1016E-10	0.7066E-11	0.6566E-11	0.3391E-11	0.4145E-11	0.2929E-22	0.2862E+03	0.9863E+06	0.4145E-04
0.200	0.8632E-11	0.8561E-11	0.6150E-11	0.5331E-11	0.2722E-11	0.4163E-11	0.2560E-22	0.2866E+03	0.9922E+06	0.4163E-04
0.150	0.7240E-11	0.7119E-11	0.5323E-11	0.4028E-11	0.2126E-11	0.4181E-11	0.2225E-22	0.2871E+03	0.9981E+06	0.4181E-04
0.100	0.6157E-11	0.5953E-11	0.4671E-11	0.2694E-11	0.1653E-11	0.4198E-11	0.1961E-22	0.2876E+03	0.1004E+07	0.4198E-04
0.050	0.5477E-11	0.5146E-11	0.4260E-11	0.1349E-11	0.1335E-11	0.4216E-11	0.1796E-22	0.2881E+03	0.1010E+07	0.4216E-04
0.000	0.5258E-11	0.4738E-11	0.4131E-11	0.1000E-24	0.1193E-11	0.4234E-11	0.1749E-22	0.2886E+03	0.1016E+07	0.4234E-04

because the mixing ratios, rather than the concentrations, have symmetric Gaussian profiles. Species F, held fixed at a 10^{-7} mixing ratio, shows a similar skewing. Species-G concentrations are established simply in terms of the noted equilibrium relationship.

Table 4-15 shows output at the end of the simulation, 3500 seconds downwind of the source, and a plot of these data is given in Figure 4-1. Species A and B differ only near the surface, because of the non-zero deposition of B. Species C and D have the same chemical reaction loss term, but the surface loss for D causes it to have a significantly lower concentration than C. The circular points on the plot denote the analytical solution of Heines and Peters (1973) for an inert, non-depositing species (i.e., species A in this example).

FIGURE 4-1. Results of Example 1 Computations at TCLOCK = 3500 Seconds
(Concentration profiles for species A through E are shown)

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5. EXAMPLE APPLICATION 2: REACTIVE SCAVENGING IN AN OROGRAPHIC STORM

This second example application of PLUVIUS simulates the precipitation scavenging of aerosols and reactive gas in an orographic storm. In this capacity, the code is also required to simulate the storm in which the scavenging processes occur. This in turn requires the additional considerations of multiphase systems and phase-transformation effects, and a moderately detailed description of the water balance.

The simulation is depicted schematically in Figure 5-1. In this figure, air is moving from left to right over a two-dimensional orographic barrier. As the air moves over the barrier, it is lifted and cooled. As a result of this cooling, cloud forms and precipitation particles (rain and snow) grow. Four pollutant species are considered in the simulation: $\text{SO}_4^=$ aerosol and gaseous SO_2 , H_2O_2 , and O_3 . The $\text{SO}_4^=$ aerosol attaches to cloud water via nucleation, resulting in water-bound "primary" $\text{SO}_4^=$ which may be scavenged subsequently by rain or snow. The gases dissolve in cloud and rain water, whereupon oxidation processes occur to generate additional "secondary" $\text{SO}_4^=$. This also may be removed by precipitation, leading to an ultimate delivery of composite sulfate to the surface.

Treatment of both the precipitation-formation processes and reactive scavenging occurs in a highly parameterized fashion. These parameterizations are discussed in some detail in the first two subsections. Following that, the input data and Class I and Class III subroutines needed for the simulation are described. Finally, output from the simulation is presented.

A. MICROPHYSICS PARAMETERIZATION

1. Water Species Classification Scheme

In real storm systems, precipitation-formation processes involve continuous spectra of liquid and solid (ice) cloud and precipitation particles ranging from micron to millimeter size and having, in the case of ice particles, complex and varying geometries and densities. Detailed treatment of the particle spectra in numerical models requires tremendous computing

FIGURE 5-1. Illustration of the Orographic Storm in Example Application 2. The heavy solid line outlines the area of cloud (cloud water $> .01 \text{ gm/m}^3$). The shaded and dotted areas show rain and snow regions (concentration $> .01 \text{ gm/m}^3$). The outline of the orographic barrier is the lighter line along the bottom (reaching maximum height of 1 km). The light line at the top shows the height of the grid top (the upper boundary of the computational domain). A time of 1 hour corresponds to a horizontal distance of 36 km.

resources, and this detail is not always justified when the cloud physics is not the main thrust of the model application. In the current application a microphysics parameterization scheme was employed which vastly reduces the complexity of simulating the precipitation processes.

The parameterization scheme follows closely the scheme initially developed by Kessler (1969) and used recently by Scott (1982a,b) in scavenging applications. Within the scheme, water substance is lumped into four categories: water vapor, cloud water, rain, and snow. The cloud water category consists of liquid particles with sizes up to several tens of microns. These cloud droplets have negligible settling velocities and essentially move with the air. The rain category consists of larger drops, with sizes in the 100- to 1,000-micron range. Both cloud water and rain are defined by single variables, their mass concentrations per volume of air denoted by M_{cloud} and M_{rain} , respectively. Within the rain category, drops have a specified size distribution. In this work (as in Kessler and Scott), a Marshall-Palmer distribution is used,

$$N_r(A)dA = N_{0,r} \cdot e^{-\lambda A} dA \quad (46)$$

where $N_r(A)dA$ is the concentration of drops with sizes (diameters) between A and $A+dA$. $N_{0,r}$ is determined empirically, and a value of $10^7 \text{ m}^{-4(a)}$ is used as per Scott (1982a). With this specification λ becomes a function of M_{rain} , since

$$M_{rain} = \int_0^{\infty} dA N(A) m(A) \quad (47)$$

where $m(A)$ is the mass of a drop with diameter A . The size distribution is used to determine mean settling velocities and mean growth rates for the rain category.

(a)For consistency with other authors, gm-m-sec units are used in this subsection. The reader should be aware that within the PLUVIUS code, mole-cm-sec units are used.

The snow category consists of all solid (ice) particles. The snow category is described by its mass concentration, M_{snow} , and within this category particles are assumed to follow a Marshall-Palmer distribution,

$$N_s(A) dA = N_{0,s} e^{-\lambda A} dA \quad . \quad (48)$$

$N_{0,s}$ is determined empirically and is allowed to vary with temperature. Based on the data from Houze et al. (1979) we employ

$$N_{0,s} = 5.6 \cdot 10^6 e^{-.088T} \quad (\text{m}^{-4}) \quad (49)$$

where T is the temperature in degrees Celsius. With this specification, λ in Equation (48) is determined by M_{snow} , as in Equation (47).

Our application of the Marshall-Palmer distribution to describe ice-particle spectra is somewhat problematic, owing to the large range of particle sizes and the diversity of growth mechanisms involved. In mid-latitude storms ice formation in upper-storm regions is usually dominated by vapor deposition to small (one-to-several hundred micron) crystals, with riming and aggregation becoming much more important as particle growth continues. Accurate description of these processes over the extended particle-size range is difficult using a simple distribution expression; we have compensated for this shortcoming by applying the Marshall-Palmer distribution throughout the total particle-size range, but making some corrective adjustments to deposition calculations involving small crystals.

The reader should note that the above treatment of the ice-phase is somewhat unconventional, and that several different microphysics parameterizations have been developed in the cloud-modeling community (e.g., Bennetts and Rawlins, 1981; Lin et al., 1983). The parameterizations differ primarily in the treatment of ice-phase cloud and precipitation particles; the parameterization used in this example application should be viewed as a highly simplified form.

2. Precipitation Formation Mechanisms

The interactions between the four water categories that eventually lead to precipitation formation are depicted in Figure 5-2. The driving force for precipitation formation is the vertical updraft, which produces adiabatic cooling and results in condensation of water vapor. Within the model, water vapor and cloud water exist at thermodynamic equilibrium. Water vapor is maintained at or below water saturation. Water vapor in excess of saturation condenses immediately to form cloud water, and cloud water evaporates immediately when water vapor falls below saturation.

Rain grows at the expense of cloud water through autoconversion and accretion. The autoconversion rate was obtained from Berry and Reinhardt (1974),

$$r_{\text{auto}} = 5.5 \cdot 10^9 (M_{\text{cloud}})^2 m_c^{5/3} \left[1 - \left(\frac{2.35 \cdot 10^{-9}}{m_c} \right)^{4/3} \right] \quad (50)$$

$$\cdot \left[1 - \left(\frac{2.04 \cdot 10^{-9}}{m_c} \right)^{1/3} \right] .$$

Here r_{auto} is in (gm/m³/sec), M_{cloud} is in gm/m³ and $m_c = M_{\text{cloud}}/n_c$ is the average cloud-drop mass (n_c is the number of cloud drops per m³). The rate of accretion of cloud drops by rain drops is taken from Scott (1982a)

$$r_{\text{accr}} = 5.2 \cdot 10^{-3} E_{\text{accr}} M_{\text{cloud}} (M_{\text{rain}})^{.875} \quad (51)$$

Here E_{accr} is the collection efficiency for water-water collisions and is set to .65 as in Scott (1982a). Below cloud base, rain is allowed to evaporate.

The evaporation rate is taken from Kessler (1969),

$$r_{\text{evap}} = 5.4 \cdot 10^{-4} \cdot (M_{\text{vapor,sat}} - M_{\text{vapor}}) \cdot (M_{\text{rain}})^{.65} \quad (52)$$

FIGURE 5-2. Interaction Diagram for Water Categories

Here $M_{\text{vapor,sat}}$ is the saturation water-vapor density and M_{vapor} is the actual water-vapor density. The rain and snow categories interact through melting and freezing. The freezing rate was obtained from Lin et al. (1983), and represents the freezing caused by collisions between raindrops and small ice crystals. The rate is

$$r_{\text{freez}} = 2.57 \cdot 10^{-5} N_u M_R^{1.63} \quad (53)$$

where N_u is the number concentration of ice crystals (m^{-3} units), taken from Scott (1982a):

$$N_u = 400 \left(-\frac{T_c}{16} \right)^4 ; \quad (54)$$

(T_c is the temperature in degrees Celsius).

The melting rate, r_{melt} , was also obtained from Lin et al. (their Equation (32), which we have chosen not to reproduce here).

The major formation mechanisms for the snow category are deposition and riming. The riming rate is evaluated, as per Scott (1982a) by integrating the growth rate over the ice particle spectrum,

$$r_{\text{rime}} = \int_0^{\infty} dA N(A) \dot{m}_{\text{rime}}(A) , \quad (55)$$

where $\dot{m}_{\text{rime}}(A)$ is the riming growth rate for an ice particle of size A . The derivation follows Scott (1982a). Scott suggests using a collection efficiency for ice-water collision of 0.1 when $A > 300\text{--}400 \mu\text{m}$ and zero for $A < 300\text{--}400 \mu\text{m}$. Using a riming cutoff of $A_0 = 350 \mu\text{m}$, the resulting integration yields

$$r_{\text{rime}} = 0.32 \cdot N_{0,s} \cdot \lambda^{-3.21} \cdot e^{-\lambda A_0} \cdot [2 + 2\lambda A_0 + (\lambda A_0)^2] \quad (56)$$

where λ and $N_{0,s}$ are from Equation (48).

The deposition growth rate also can be evaluated by integrating the individual crystal growth rates over the ice-particle spectrum using the Marshall-Palmer distribution. In the ice-formation zone near the cloud tops, however, this method seriously underestimates the growth rate. The reason is that the Marshall-Palmer distribution most accurately describes the spectrum of large ice particles, and it underestimates the number of ice particles when M_{snow} is small. This in turn causes the depositional growth rate to be underestimated. To remedy this, the depositional growth rate was calculated using a second method. In this alternative procedure, the ice particles are assumed to be uniform in size, and have a number concentration given by Equation (54). The deposition growth is then

$$r_{\text{dep},u} = N_u \cdot \dot{m}_{\text{dep}}(A_u) \quad (57)$$

where $\dot{m}_{\text{dep}}(A_u)$ is the deposition growth rate of an individual ice particle with size A_u and mass (M_{snow}/N_u). The individual crystal growth rates, $\dot{m}_{\text{dep}}$, were taken from Scott.

The Marshall-Palmer deposition growth rate, $r_{\text{dep},mp}$ was evaluated using the individual crystal growth rates from Scott (1982a) and

$$r_{\text{dep},mp} = \int_0^{\infty} dA N(A) \dot{m}_{\text{dep}}(A) \quad (58)$$

Because the individual crystal growth rate is roughly proportional to the crystal size A , we have

$$r_{\text{dep},mp} = N_T \cdot \dot{m}_{\text{dep}}(\bar{A}) \quad (59)$$

where $\bar{A}$ is the average crystal size ($\bar{A}=1/\lambda$) and N_T is the total number of crystals given by the Marshall-Palmer distributions. However, Equation (59) presents the problem that when M_{snow} is large it may predict $N_T > N_u$, which is unrealistic. We thus define N_T^* as the smallest of N_T and N_u and define $\bar{A}^*$ such that

$$N_T^* = \int_{A^*}^{\infty} dA N(A) . \quad (60)$$

It should be noted here that A^* is zero if $N_T^* = N_T$. We then define

$$r_{\text{dep},\text{mp}^*} = \int_{A^*}^{\infty} dA N(A) \dot{m}_{\text{dep}}(A) , \quad (61)$$

which gives

$$r_{\text{dep},\text{mp}^*} = N_T^* \cdot \dot{m}_{\text{dep}}(\bar{A}^*) , \quad (62)$$

where $\bar{A}^* = (A^* + 1/\lambda)$. The value of r_{dep} used in the model is now chosen to be the largest of $r_{\text{dep},u}$ and $r_{\text{dep},\text{mp}^*}$.

3. Precipitation Fallspeeds

The fallspeeds for rain and snow categories are simply the average mass-weighted fallspeed obtained using the Marshall-Palmer distribution, e.g.

$$v_{\text{rain}} = \frac{\int_0^{\infty} dA N(A) m(A) v(A)}{M_{\text{rain}}} \quad (63)$$

Based on previous work by Kessler (1969) and by Pruppacher and Klett (1978) we have applied the following expressions for evaluation of Equation (63) in the case of rain:

$$v(A) = 130 A^{1/2} \quad A > 10^{-3} \text{ m} \quad (64a)$$

$$v(A) = 4055 A \quad A < 10^{-3} \text{ m} \quad (64b)$$

Similarly, in evaluating v_{snow} , we have used

$$v(A) = 3.33 A^{.206} \quad A > 10^{-3} m \quad (65a)$$

$$v(A) = 473 A^{.927} \quad A < 10^{-3} m \quad (65b)$$

where Equation (65a) is from Scott (1982a) and Equation (65b) is from Scott (1976).

B. CHEMISTRY PARAMETERIZATION

As noted earlier, the chemistry in this second example application is limited to four pollutant species: sulfate aerosol and gaseous SO_2 , O_3 , and H_2O_2 . The intent is not to provide a rigorous simulation of reactive SO_2 chemistry. Rather, this example was chosen to provide an instructive demonstration of reactive and non-reactive gas scavenging and aerosol scavenging using the PLUVIUS code. The extension of this example to a more elaborate chemical mechanism (both gas and aqueous phase) simply requires the inclusion of more species in the simulation; difficulties arise mainly from specifying reaction rates, solubilities, dissociation constants, and other physical parameters.

The treatment of chemistry is closely linked to the microphysical parameterization. For each pollutant species, one must consider that species associated with each water category. Thus, besides gaseous SO_2 , one must treat SO_2 dissolved in cloud water, in rain, and in snow. The dependent variables needed for this example are summarized in Table 5-1. Several points should be noted concerning this table. First, for SO_2 , H_2O_2 , and water itself, the sum of the gas-phase concentration and cloud water associated concentration is treated as a single computed variable (e.g., KS02GC, KH202GC, KVAPCL), while the concentrations are treated individually as constrained species (KS02G and KS02C, etc.). This combination is possible because the two "phases" are in equilibrium, and also move with the same vertical velocities. A similar treatment is possible for O_3 . However, the low solubility of O_3 makes it possible to treat both the O_3 in cloud and in rain by equilibrium solubility and simply compute these concentrations as temporary variables when needed.

The different phases for each pollutant species lead to a multitude of possible pathways which transfer mass between the different variables: mass

TABLE 5-1. Dependent Variables for Example Application 2

<u>Variable</u>	<u>Species Location Variable</u>	<u>Type</u>
Temperature	KTEMP	Computed
Water Vapor and Cloud Water	KVAPCL	Computed
Rain	KRAIN	Computed
Snow	KSNOW	Computed
Cloud Water	KCLOUD	Constrained by Saturation Equilibrium
Sulfate Aerosol	KS04A	Computed
Sulfate in Cloud Water	KS04C	Computed
Sulfate in Rain	KS04R	Computed
Sulfate in Snow	KS04S	Computed
SO ₂ in Gas Phase and in Cloud Water	KS02GC	Computed
SO ₂ in Rain	KS02R	Computed
SO ₂ in Snow	KS02S	Computed
SO ₂ in Cloud Water	KS02C	Constrained by Solubility Equilibrium
SO ₂ in Gas Phase	KS02G	Constrained by Solubility Equilibrium
H ₂ O ₂ in Gas Phase and in Cloud Water	KH202GC	Computed
H ₂ O ₂ in Rain	KH202R	Computed
H ₂ O ₂ in Snow	KH202S	Computed
H ₂ O ₂ in Cloud Water	KH202C	Constrained by Solubility Equilibrium
H ₂ O ₂ in Gas Phase	KH202G	Constrained by Solubility Equilibrium
Gas Phase O ₃	K03G	Computed
H ⁺ in Cloud Water	KH10NC	Constrained by Empirical Relation
H ⁺ in Rain	KH10NR	Constrained by Empirical Relation

transfer of gases and aerosol to liquid phases, transfer between phases by the precipitation-formation processes, and chemical reaction in each phase. These pathways are summarized for sulfur species in the interaction diagram shown in Figure 5-3. The paths between gaseous SO_2 and cloud or rain SO_2 represent mass transfer. The paths between aerosol SO_4 and cloud or rain SO_4 represent aerosol scavenging or evaporation. The paths between cloud, snow, and rain phases of each species represent precipitation processes. The paths between SO_2 and SO_4 represent aqueous chemical reactions.

The multiphase nature of the present example again should be stressed. Example Application 1 involved clear air and homogeneous chemistry; and pollutant concentrations were denoted by c , the moles of pollutant per cubic-centimeter space. In the present example, however, there are several different media to choose for volumetric bases. In liquid-phase reaction-rate calculations, for example, one may desire to express concentration in terms of moles per cubic centimeter liquid, whereas gas-phase calculations normally are conducted on a gas-volume basis. To preserve consistency in PLUVIUS we shall *always* describe the dependent variable, c , in terms of moles per unit volume *total space* (volume of gas and liquid water and ice and . . .). Likewise, chemical reaction rates [G_k in Equation (1) and GGEN and GDEC in the code], shall always be expressed in units of moles per second per unit volume total space.

It is convenient in the following discussion to use other volumetric bases on occasion. When doing this we employ the following nomenclature:

c	moles pollutant per cubic centimeter total space
$\hat{c}$	moles pollutant per cubic centimeter of chosen condensed phase (liquid water, ice, ...)
$\tilde{c}$	moles pollutant per liter of chosen condensed phase
G_k	moles pollutant per second per cubic centimeter total space
$\hat{G}_k$	moles pollutant per second per cubic centimeter condensed phase

FIGURE 5-3. Interaction Diagram for Sulfur Species

In making his own applications, the reader is well advised to exercise due care in distinguishing between these various definitions of concentration. It is relatively easy to mix definitions inadvertently in such endeavors; and once made, such errors often are highly difficult to detect and/or resolve.

1. Aerosol Scavenging

In the computations performed for this example, the in-cloud scavenging of sulfate aerosol is presumed to occur totally via a nucleation mechanism. This is expected to be an appropriate first approximation, owing to the secondary importance of competitive mechanisms, such as diffusional and phoretic processes, for particles in this size range. Cloud-droplet number density is set within PLUVIUS to a value typical of continental cloud systems (500 nuclei/cm^3) and, at the instant of cloud formation, this number of sulfate particles is incorporated into the droplet phase. New sulfate particles are allowed to nucleate within the modeled system as the sulfate-containing droplets are removed by conventional rain-formation processes. For the present application, the sulfate-aerosol size distribution is presumed to be monodisperse, with a particle diameter of $0.3 \text{ }\mu\text{m}$.

As can be noted from Figure 5-3, sulfate aerosol can be reinjected to the gaseous medium by evaporation of cloud droplets. Secondary sulfate (that is, that which has been formed by in-cloud conversion) is treated in a manner identical to "primary" sulfate once it has been reinjected in this fashion. For the present example, the size of the reinjected particles is taken to be the same as those of the original sulfate aerosol.

2. Nonreactive Gas Scavenging

In this example, the so-called "equilibrium scavenging" assumption for dissolved SO_2 and H_2O_2 in cloud water and for dissolved O_3 in cloud water and rain. This assumption has been demonstrated valid for cloud water (high surface to volume ratio), and for rain with gases at low solubility (O_3). For dissolved SO_2 and H_2O_2 in rain, the mass transfer is calculated explicitly.

SO₂ and H₂O₂ in snow result only from the transfer of the cloud or rainborne species to snow; no direct gas-to-snow transfer is treated in this example.

For ozone and H₂O₂, equilibrium scavenging means that the aqueous concentrations are determined simply on the basis of solubility equilibrium. The solubility relation for O₃ used here is from Kirk and Othmer (1947):

$$\hat{c}_{O_3|aq} = .45 c_{O_3|g} \quad (66)$$

The solubility relation for H₂O₂ is from Schumb et al. (1955):

$$\tilde{c}_{H_2O_2|aq} = 6.763 \cdot 10^{-4} T e^{6834.93/T} c_{H_2O_2|g} \quad (67)$$

For SO₂, the treatment is more involved, since the dissociation of aqueous SO₂ must be considered.^(a) The relation used here is given by Hales and Sutter (1973):

$$y_{SO_2} = H' \hat{c}_{SO_2|e} \quad (68)$$

$$H' = \frac{y_{SO_2}}{\left(y_{SO_2}/H_0 - (\tilde{c}_{H^+} - \sqrt{\tilde{c}_{H^+}^2 + 4 y_{SO_2} K_1/H_0})/2 \right)} \quad (69)$$

$$H_0 = \exp (10.21 - 3112./T)/P, \text{ and}$$

$$K_1 = \exp (-10.96 + 1970./T) ,$$

where y_{SO_2} = mole fraction of SO₂ in gas phase (= c_{SO_2}/c_{air})

$\hat{c}_{SO_2}$ = concentration of S^{IV} in aqueous phase, (moles/cm³ water)

(a) "Dissolved SO₂" in this report will be taken to be the sum of all ionic and undissociated species existing in the +4 valence state.

$\tilde{c}_{H^+}$ = aqueous-phase hydrogen-ion concentration contributed from species other than dissolved SO_2 , molar

T = temperature, K

P = pressure, atm.

It is important to note in the context of the above relationships that H_{ex} is important in determining the solubility of SO_2 , and thus its rate of nonreactive scavenging. If a more detailed treatment of aqueous chemistry were being used, then the hydrogen-ion concentration could be calculated directly using the electro-neutrality condition. For present purposes, hydrogen-ion concentrations in cloud water and rainwater are determined on the basis of concurrently-existing sulfate concentrations, using the empirical form

$$\tilde{c}_{H^+} = 1.03 \times 10^{-5} + 1.184 \left(\tilde{c}_{SO_4} \right), \text{ molar} \quad (72)$$

which has been derived from regional precipitation chemistry data (MAP3S/RAINE, 1982). With this treatment, cloud and rain acidity are treated as individual *constrained* variables in the code.

For the scavenging of SO_2 and H_2O_2 by rain, the mass-transfer rates computed by Levine and Schwartz (1982) for Marshall-Palmer raindrop distributions have been used. This results in an expression of the form

$$\frac{d}{dt} \left(c_{SO_2|rain} \right) = - \frac{d}{dt} \left(c_{SO_2|gas} \right) = \Lambda \cdot \left(c_{SO_2|gas} - c_{SO_2|equilib} \right). \quad (73)$$

Here $c_{SO_2|equilib}$ is the gas-phase SO_2 concentration that would be in equilibrium with the dissolved SO_2 in the rain, and is calculated by applying Equation (68)-(69); Λ is obtained from Levine and Schwartz. A similar rate expression results for H_2O_2 .

3. Aqueous Phase Chemical Transformation

Two chemical reactions involving dissolved SO_2 and H_2O_2 or O_3 are treated in the example. The reactions convert dissolved SO_2 (S^{IV}) to dissolved sulfate (S^{VI}) both in the cloud water and in the rain water. No chemical reactions are considered in the gas or snow phases.

The rate expression for the SO_2 - O_3 reaction is derived from the results of Penkett et al. (1979):

$$\begin{aligned} \text{rate of sulfate generation} &= \frac{2.9\text{E6}}{\sqrt{\hat{c}_{\text{H}^+}}} \hat{c}_{\text{O}_3} \hat{c}_{\text{SO}_2} \\ (\text{units} &= \text{moles/cm}^3 \text{ water} \cdot \text{sec}) \end{aligned} \quad (74)$$

Here $\hat{c}_{\text{H}^+}$ is the hydrogen-ion concentration (molar), which is approximated by Equation (72).

The rate expression for the SO_2 - H_2O_2 reaction is derived from Martin and Damschen (1981):

$$\begin{aligned} \text{rate} &= \frac{4.6\text{E7 } c_{\text{H}_2\text{O}_2|\text{aq}} c_{\text{SO}_2|\text{aq}}}{c_{\text{water}} \left[1 + \frac{K_1}{\hat{c}_{\text{H}^+}} \left(1 + \frac{K_2}{\hat{c}_{\text{H}^+}} \right) \right]} \\ (\text{units} &= \text{moles/cm}^3 \text{ water} \cdot \text{sec}) \end{aligned} \quad (75)$$

where K_1 and K_2 are the first and second dissociation constants for aqueous SO_2 , and c_{water} is either c_{rain} or c_{cloud} as appropriate.

C. INPUT DATA

Input data for this example are given in Table 5-2, and they should be compared with the input statements described in Section 3. The first input line is a run title which will appear on the printed output. The second input line specifies that there are 15 computed variables and 7 constrained variables in the example. The next 22 input lines provide names for each variable, for use during program output.

TABLE 5-2. Input Data for Example Application 2

Line	Data									
1:	EXAMPLE RUN 2 - PLUVIUS MOD 5.0 USER MANUAL									
2:	15	7								
3:	TEMP									
4:	VAPCL									
5:	RAIN									
6:	SNOW									
7:	S02-GC									
8:	S02-R									
9:	S02-S									
10:	S04-A									
11:	S04-C									
12:	S04-R									
13:	S04-S									
14:	H202-GC									
15:	H202-R									
16:	H202-S									
17:	O3-G									
18:	CLOUD									
19:	HION-C									
20:	HION-R									
21:	S02-G									
22:	S02-C									
23:	H202-G									
24:	H202-C									
25:	26	4	0.2E5	0.0						
26:		0.	14400.	60.						
27:	0	3600.	1	180.						
28:	1	1	1	1	1	0	1	1	0	
29:	1	1	1		0.					
30:	1	1	2		0.					
31:	1	-1	3	.10						
32:	1	-1	4	.10						
33:	1	1	2		0.					
34:	1	-1	3	.10						
35:	1	-1	4	.10						
36:	1	1	2		0.					
37:	1	1	2		0.					
38:	1	-1	3	.10						
39:	1	-1	4	.10						
40:	1	1	2		0.					
41:	1	-1	3	.10						
42:	1	-1	4	.10						
43:	1	1	2		0.					
44:	1.0E6	288.15								

Input line 25 specifies that the vertical grid consists of 26 grid points, that there are four "diffusion regimes", that the uniform grid spacing is $2 \cdot 10^4$ cm (.2 km), and that the initial height of the bottom grid point (GLEVL) is at 0 cm. Input line 26 specifies that the simulation begins at a time of 0 seconds, terminates at a time of 14,400 seconds (4 hours), and uses an initial integration time step of 60 seconds. Input line 27 specifies output control information. As NPRINT is zero and DTPRIN is positive (3600), printed output will occur every 3600 seconds. The ITCOLL and DTCOLL values (1 and 180) specify that output to disk file will occur each 180 seconds, and this output will be time-averaged over the 180-second intervals.

Input line 28 specifies the bypass variables. All but IBOUND and ISHEAR are 1. Thus the BOUND and USHEAR routines will only be called once during initialization. The other Class I routines with bypass variables will be referenced throughout the simulation.

Input lines 29 through 43 specify the boundary conditions, diffusion regimes, and filter factors for each of the 15 computed species. All of the top boundary conditions are flux-specified (ITOP = 1). The rain- and snow-associated species have outflow bottom-boundary conditions (IBOT = -1), and filter factors of 0.1. These species have significant settling velocities, so the outflow boundary condition is appropriate; these settling velocities also result in the need to apply the smoothing filter after the advection-diffusion integration steps. The other species, which have zero settling velocities, have flux-specified bottom boundary conditions (IBOT = 1) and do not require filtering (FILFAC = 0). The rain- and snow-associated species use diffusion regimes 3 and 4, respectively. Temperature uses regime 1, and all remaining species use regime 2. The final input line specifies initial surface pressure and temperature.

D. CLASS I SUBROUTINE DESCRIPTIONS

As discussed in Section 3, the ten Class I subroutines are the primary mechanism by which the physics and chemistry appropriate to a particular application are inserted into the PLUVIUS framework, and it is extremely important that the user have a good understanding of each. The listings and discussions of these subroutines for the second example application should provide additional insight about them.

SUBROUTINE SETUP (Table 5-3)

SETUP defines the initial concentration profiles for the dependent variables and state variables, and also defines the species location variables. The species location variables for the 22 computed and constrained variables of this example are defined in the initial data statements. Note again that these values must correspond exactly to the ordering of species given in the input data (in this case, temperature is first and H_2O_2 in cloud water is last). The next statements specify values used in the ODEINT subroutine. Note that CMIN and CERROR are larger for temperature and water species than for pollutant species. Making these variables too small may impose unnecessary constraints on the integrator, while making them too large can result in an inaccurate solution. Values should be chosen which are small in comparison to significant values of each species, but not "too small."

The first executable statements compute the initial temperature and pressure profiles. For this example, we have arbitrarily chosen a moist-adiabatic temperature profile. A rough temperature profile (lapse rate = $7^\circ/\text{km}$) is first computed, so that approximate pressure and density profiles can be set. Next, the moist adiabatic temperature profile is computed, using the Class II subroutine RLAPSE, and another PRESSF call recomputes the pressure and density profiles.

Next, the water vapor profile is established. It is arbitrarily set at 90% relative humidity for this example. Finally, the other variables are initialized. The only non-zero variables are aerosol sulfate and gaseous SO_2 , H_2O_2 , and O_3 . O_3 is set to 50 ppb. SO_2 , H_2O_2 , and sulfate are set to 10 ppb, 1 ppb, and 1 ppb, respectively, below 1.5 km altitude, and 1/5 these values above 1.5 km.

Table 5-4 shows the common blocks in the INCLUDE file PLUVCMN for this example. The differences between this and example 1 are:

- The LOCATN common block holds the appropriate species location variables.
- Arrays are dimensioned to appropriate sizes (via the NZMAX, NCMAX, and NCTMAX parameters).

TABLE 5-3. Listing of Subroutine SETUP for Example Application 2

```

SUBROUTINE SETUP

  INCLUDE 'PLUVCMN'

C
C ESTABLISH SPECIES LOCATION VARIABLE VALUES
C
      DATA KTEMP, KVAPCL, KRAIN, KSNOW, KCLOUD/1,2,3,4,16/
      DATA KS02GC,KS02R,  KS02S, KS02G, KS02C/5,6,7,19,20/
      DATA KS04A, KS04C,  KS04R, KS04S/8,9,10,11/
      DATA KH202GC,KH202R, KH202S, KH202G, KH202C/12,13,14,21,22/
      DATA K03G/15/
      DATA KHIONC, KHIONR/17,18/

C
C ESTABLISH PARAMETERS USED IN O.D.E. INTEGRATION ROUTINE (ODEINT)
C
      DATA EPS / .01 /
      DATA DTMIN / 1.E-10 /
      DATA RATESF / NCMAX*1.E-2 /
      DATA NCORR / 1 /
      DATA IEXP / 1 /

      DATA CMIN / NCTMAX*1.E-24 /
      CMIN(KTEMP) = 1.E-8
      CMIN(KVAPCL) = 1.E-17
      CMIN(KRAIN) = 1.E-17
      CMIN(KSNOW) = 1.E-17
      CMIN(KCLOUD) = 1.E-17

      DO K = 1, NCOMP
        CERROR(K) = CMIN(K)*1.E4
      END DO

C
C ZERO OUT ALL CONCENTRATIONS
C
      DO I = 1, N
        DO K = 1, NTOT
          C(I,K)=0.
        END DO
      END DO

C
C ESTABLISH TEMPERATURE, DENSITY, AND PRESSURE FIELDS
C FOR THIS EXAMPLE, TEMPERATURE FOLLOWS MOIST ADIABAT
C
C USE CONSTANT LAPSE RATE TO GET ROUGH PROFILE

```

TABLE 5-3 Continued

```

DO I = 1, N
  C(I,KTEMP) = TEMP0 - 7.E-5*(Z(I)-Z(1))
END DO
CALL PRESSF( 1 )

C
C NOW USE MOIST ADIABATIC LAPSE RATE
TEMP = TEMP0
DO I = 2, N
  TEMP = TEMP + (Z(I)-Z(I-1))*RLAPSE( TEMP, CS(I-1), 1 )
  C(I,KTEMP) = TEMP
END DO
CALL PRESSF( 0 )

C
C ESTABLISH WATER VAPOR PROFILE - 90% RH
C
DO I = 1, N
  C(I,KVAPCL) = 0.9*SAT( C(I,KTEMP) )
END DO

C
C ESTABLISH INITIAL CONCENTRATIONS OF OTHER SPECIES
C
DO I = 1, N
  ONEPPB = 1.E-9*CS(I)
  IF (Z(I) .LE. 1.5E5) THEN
    C(I,KS02GC) = 10.*ONEPPB
    C(I,KS04A) = ONEPPB
    C(I,KH2O2GC) = ONEPPB
  ELSE
    C(I,KS02GC) = 2.*ONEPPB
    C(I,KS04A) = 0.2*ONEPPB
    C(I,KH2O2GC) = 0.2*ONEPPB
  END IF
  C(I,KO3G) = 50.*ONEPPB
END DO

RETURN
END

```

TABLE 5-4. Example Listing of PLUVIUS Common Blocks
(held in the PLUVCMN INCLUDE file)
for Example Application 2

```

PARAMETER ( NZMAX=26 )      ! NO. OF VERTICAL GRID POINTS
PARAMETER ( NCMAX=15 )      ! NO. OF "COMPUTED" VARIABLES
PARAMETER ( NCTMAX=25 )      ! NO. OF COMPUTED+CONSTRAINED VARIABLES

PARAMETER ( NNAMMX= NCTMAX+2 )
PARAMETER ( LUNIN=5, LUNOUT=6 )

COMMON /NAMES/ NAME(5,NNAMMX), MTITLE(40)

COMMON /PLUV/ COLD(NZMAX,NCTMAX), C(NZMAX,NCTMAX),
+   WR(NZMAX,NCMAX), WAP(NZMAX), WAGRID(NZMAX), D(NZMAX,4),
+   URATIO(NZMAX), LDIF(NCMAX), ITOP(NCMAX), IBOT(NCMAX),
+   FT(NCMAX), FB(NCMAX), CT(NCMAX), CB(NCMAX),
+   LTD, NCOMP, NCNSTR, NTOT, IGEN, IDIFF,
+   ITEMP, IPRESS, ISETTL, IBOUND, IVERT, IFOG, ISHEAR

COMMON /GRID/ N, NM1, DZ, DT, DTOLD, TCLOCK, TNEXT,
+   Z(NZMAX), GLEVL

COMMON /CHEM/ CNN(NCTMAX), GGEN(NCTMAX), GDEC(NCTMAX),
+   CMIN(NCTMAX), DTSAVE(NZMAX)

COMMON/ODEINT/ NCORR, IEXP, EPS, DTMIN, RATESF(NCMAX),
+   CERROR(NCMAX)

COMMON /THERMO/ PRESS(NZMAX), CS(NZMAX), CPCSPS(NZMAX),
+   ISSAT(NZMAX), TEMP0, PRESS0

COMMON /LOCATN/ KTEMP, KVAPCL, KRAIN, KSNOW, KCLOUD,
+   KS02GC, KS02R, KS02S, KS02G, KS02C,
+   KS04A, KS04C, KS04R, KS04S,
+   KHIONC, KHIONR, K03G,
+   KH202GC, KH202R, KH202S, KH202G, KH202C,

COMMON / ADVDIF / ADIFFU(NZMAX,4), BDIFFU(NZMAX,4),
+   CDIFFU(NZMAX,4), DZDIZ(NZMAX), FTOLD(NCMAX), FBOLD(NCMAX),
+   WVAR(NZMAX), DWVCDI(NZMAX),
+   C1(NZMAX), C1DWAP(NZMAX), C1DLCS(NZMAX), D1ADV(NZMAX),
+   AMAT(2,2,NZMAX), BMAT(2,2,NZMAX), CMAT(2,2,NZMAX),
+   DVEC(2,NZMAX), UVEC(2,NZMAX)

```

SUBROUTINE ADJUST (Table 5-5)

ADJUST performs three functions in the example. First, it treats nucleation scavenging of sulfate aerosol if cloud has just formed at a grid point. (To do this it must also compute the new cloud-water concentration, which it does initially). Second, if cloud has just evaporated, any remaining sulfate in cloud water is transferred to aerosol sulfate. Last, if the temperature is warmer than 5 C, it converts any snow or snowborne species to rain and rainborne species. This is done to "clean up" insignificantly small concentrations which are numerical artifacts of the advection scheme.

SUBROUTINE BOUND (Table 5-6)

BOUND provides values for flux or concentration specified boundary conditions. For this example, the top boundary is treated as impervious, and all the species have a flux boundary condition with zero flux at the top. At the bottom boundary, we are artificially using a zero flux condition for the gas, aerosol, and cloud type species. The rainborne and snowborne species have outflow bottom boundary conditions, because they have significant settling velocities. Note that the code zeroes FB, the bottom flux, for all variables: the FB has no effect on the outflow boundary condition variables, so it is convenient to just zero all the FB's rather than doing it selectively.

Because the values of FT and FB are not time dependent, BOUND only needs to be called once, during initialization, so the bypass variable IBOUND is set to zero.

SUBROUTINE DIFF (Table 5-7)

DIFF sets the vertical eddy diffusivities for each diffusion regime. In this example, four regimes are used. Regime 1 is for temperature (i.e., heat), Regime 2 is for gases, aerosols, and cloudborne species. Regime 3 is for rain and rainborne species and Regime 4 is for snow and snowborne species.

The actual eddy diffusivity is $10^5 \text{ cm}^2/\text{sec}$ for each regime in this example. For rain and snow, a "pseudo-diffusivity" is added on to parameterize the vertical dispersion of precipitation, which results from the variation of settling velocity with particle size. This pseudo-diffusivity is given by

TABLE 5-5. Listing of Subroutine ADJUST for Example Application 2

```

SUBROUTINE ADJUST

INCLUDE 'PLUVCMN'

DATA XNC / 500. /      ! CLOUD DROP CONC. (NO./CM**3)
DATA DPS / 0.3E-4 /    ! AEROSOL DIAMETER (CM)

DO 1000 I = 1,N

C
C  CALC NEW CLOUD CONC
C
    TEMP = C(I,KTEMP)
    CLDOLD = C(I,KCLOUD)
    CLOUD = AMAX1( 0., C(I,KVAPCL)-SAT(TEMP) )
    C(I,KCLOUD) = CLOUD

C
C  AEROSOL PICKUP BY NUCLEATION IF NEW CLOUD HAS FORMED
C    XNSO4A = NO. OF SULFATE PARTICLES PER CM**3
C
    IF ((CLOUD.GT.CMIN(KCLOUD)) .AND.
+      (CLDOLD.LE.CMIN(KCLOUD))) THEN
        CSO4A = AMAX1(0., C(I,KS04A))
        XNSO4A = CSO4A/(.0053*(DPS**3))
        IF (XNC .LT. XNSO4A) THEN
            FRACNU = XNC/XNSO4A
        ELSE
            FRACNU = 1.
        END IF
        CSNUC = CSO4A*FRACNU
        C(I,KS04C) = C(I,KS04C) + CSNUC
        C(I,KS04A) = C(I,KS04A) - CSNUC

C
C  AEROSOL RELEASE IF THERE IS NO CLOUD
C
        ELSE IF (CLOUD .LE. CMIN(KCLOUD)) THEN
            C(I,KS04A) = C(I,KS04A) + C(I,KS04C)
            C(I,KS04C) = 0.

        END IF

C

```

TABLE 5-5 Continued

```
C   FOR TEMP > 5 C, MELT SNOW AND TRANSFER SNOWBORNE SPECIES TO RAIN
C
      IF (TEMP .GE. 278.15) THEN
        C(I,KRAIN) = C(I,KRAIN) + C(I,KSNOW)
        C(I,KSNOW) = 0.
        C(I,KS02R) = C(I,KS02R) + C(I,KS02S)
        C(I,KS02S) = 0.
        C(I,KS04R) = C(I,KS04R) + C(I,KS04S)
        C(I,KS04S) = 0.
        C(I,KH202R) = C(I,KH202R) + C(I,KH202S)
        C(I,KH202S) = 0.
      END IF
1000 CONTINUE

      RETURN
      END
```

TABLE 5-6. Listing of Subroutine BOUND for Example Application 2

```
      SUBROUTINE BOUND (INIT)
      INCLUDE 'PLUVCMN'
C
C   FOR FLUX B.C., PLACE APPROPRIATE FLUX IN FT(K) OR FB(K)
C   FOR CONC. B.C., PLACE APPROPRIATE CONC. IN CT(K) OR CB(K)
C   FOR OUTFLOW B.C., DO NOTHING HERE
C
      DO K = 1, NCOMP
         FT(K) = 0.
         FB(K) = 0.
      END DO

      RETURN
      END
```

TABLE 5-7. Listing of Subroutine DIFF for Example Application 2

```

SUBROUTINE DIFF (INIT)
C
C   DIFF COMPUTES VERTICAL EDDY DIFFUSIVITIES FOR EACH DIFFUSION REGIME
C
  INCLUDE 'PLUVCMN'

  DO 1000 I = 1,N

    D(I,1) = 1.E5
    D(I,2) = 1.E5

C
C   FOR RAIN, CALCULATE A PSEUDO-DIFFUSION TERM TO
C   SIMULATE THE SPATIAL DISPERSION WHICH RESULTS FROM
C   RAIN DROP POPULATION HAVING VARYING FALLSPEEDS
C
    XRAIN = AMAX1(0.,C(I,KRAIN))*1.8E7
    DSPRED = DT*1.714*(XRAIN**.25)/1.0E-4
    D(I,3) = 1.E5 + DSPRED

C
C   SIMILARLY FOR SNOW
C
    XSNOW = AMAX1(0.,C(I,KSNOW))*1.8E7
    TEMPC = C(I,KTEMP)-273.15
    Y0FLAK = 5.681E6*EXP(-0.0878*AMIN1(TEMPC,0.))
    SLAMBD = 5.63*(Y0FLAK/(XSNOW+1.E-20))**.3333
    AFLAKE = 1./SLAMBD
    VBARG = 3.33*(AFLAKE**.206)*.155
    IF (AFLAKE.LT.4.6E-5) VBARG = 473.0*(AFLAKE**.927)*1.47
    DSPRED = DT*VBARG*VBARG/1.0E-4
    D(I,4) = 1.E5 + DSPRED

1000  CONTINUE
      RETURN
      END

```


$$D_{\text{pseudo}} = \Delta t \cdot (\overline{v^2} - \bar{v}^2)$$

where Δt is the integration time interval, $\overline{v^2}$ is the mass-weighted average of the square of the settling velocity (over the Marshall-Palmer size distribution), and $\bar{v}$ is the mass-weighted average of the settling velocity. D_{pseudo} is calculated using Equation (64) and (65), and the result is coded into DIFF in Table 5-6.

Because these pseudo-diffusivities are concentration dependent and change with time, IDIFF has been set equal to 1.

SUBROUTINE GEN (Table 5-8)

GEN computes the generation and decay rates for the computed species, and also sets constrained species. In this example, GEN is the largest of the Class I subroutines because it implements most of the cloud physics and chemistry parameterizations discussed in the first two parts of this chapter.

At the start of the subroutine, several widely used species values are stored in local variables (temperature, rain, snow, cloud, water vapor), and the constrained variable cloud-water is calculated, using the water-vapor saturation constraint. This is followed by the section that computes cloud physics generation and decay rates. Note that many of these rates are expressed as pseudo first-order rates (e.g., ACCR, RIM, SMEL) with units of sec^{-1} , so that they may also be used to compute generation and decay terms for the waterborne pollutant species resulting from the same cloud physics process. Several rates for decay processes (SMEL, FREEZ, EVAP, SUBLIM) have been arbitrarily limited to a maximum value of 1 sec^{-1} . This has been done to improve computational efficiency (reduce stiffness). (The limit of 1 sec^{-1} does not significantly affect the solution, although a lower limit, say 0.01 sec^{-1} , could have significant effects.)

The next section computes constrained species (besides cloud water). This involves the equilibrium relations

TABLE 5-8. Listing of Subroutine GEN for Example Application 2

SUBROUTINE GEN (I, IGCALC, TGEN, DTAU, JPASSO)

```

C
C  I = VERTICAL GRID INDEX AT WHICH GEN/DECAY RATES ARE TO BE COMPUTED
C  IGCALC = IF 0, ONLY CALCULATE CONSTRAINED VARIABLES
C  TGEN = CURRENT MODEL TIME
C  DTAU = CURRENT INTEGRATION TIME STEP IN O.D.E. INTEGRATOR
C  JPASSO = FLAG SPECIFYING PREDICTOR (1) OR CORRECTOR (2,3,...) PASS
C          IN O.D.E. INTEGRATOR
C
      INCLUDE 'PLUVCMN'

      DATA XNC /500./
      DATA DPS /0.3E-4/

      DO K = 1, NCOMP
         GGEN(K) = 0
         GDEC(K) = 0.
      END DO

C
C  DEFINE LOCAL WATER AND TEMPERATURE VARIABLES
C  CALCULATE NEW CLOUD AND WATER VAPOR
C  CALCULATE WATER VAPOR SATURATION CONCENTRATIONS
C
      TEMP = CNN(KTEMP)
      TEMPC = TEMP-273.15
      VSATW = SAT( TEMP )
      VAPOR = AMIN1( CNN(KVAPCL), VSATW )
      CLOUD = CNN(KVAPCL) - VAPOR
      CNN(KCLOUD) = CLOUD
      RAIN = CNN(KRAIN)
      SNOW = CNN(KSNOW)

      IF (TEMPC .LE. 0.) THEN
         VSATI = SSAT( TEMP )
      ELSE
         VSATI = VSATW
      END IF

C-----
C
C  CLOUD PHYSICS - CALCULATE GENERATION AND DECAY RATES FOR WATER SPECIES
C-----
C  X---- VARIABLES ARE CONCENTRATIONS IN GM/M**3
C

```

TABLE 5-8 Continued

```

XCLOUD = CLOUD*1.8E7
XRAIN = RAIN*1.8E7
XSNOW = SNOW*1.8E7
XVAPOR = VAPOR*1.8E7
AUTO = 0.
ACCR = 0.
EVAP = 0.
FREEZ = 0.
SMEL = 0.
RIM = 0.
DEPOSI = 0.
SUBLIM = 0.

C
C AUTOCONVERSION RATE = AUTO*CLOUD
C ACCRETION RATE = ACCR*CLOUD
C
  IF (CLOUD .GT. 0.) THEN
    XCDROP = XCLOUD/(XNC/1.0E-6)
C    XCDROP = (CLOUD WATER MASS CONC.)/(CLOUD DROPLET NUMBER CONC.)
    IF (XCDROP.GT.2.348E-9) AUTO = 5.504E9*XCLOUD*
      1 (XCDROP**1.667)*(1.-(2.347E-9/XCDROP)**1.333)*
      2 (1.-(2.040E-9/XCDROP)**.333)
    ACCR = 3.39E-3*(XRAIN**.875)
  ELSE
C
C EVAPORATION RATE = EVAP*RAIN
C
    EVAP = 5.44E-4*(VSATW*1.8E7-XVAPOR)/
      1 (AMAX1(XRAIN,1.E-25)**.35)
    EVAP = AMAX1(0.,EVAP)
    EVAP = AMIN1( 1.0, EVAP )
  END IF

C
C RIMING GROWTH RATE = RIM*CLOUD
C Y0FLAK = N0,S FROM MARSHALL-PALMER DISTRIBUTION
C SLAMBD = LAMBDA FROM MARSHALL-PALMER DISTRIBUTION
C
Y0FLAK = 5.681E6*EXP(-.0878*AMIN1(TEMPC,0.))
SLAMBD = 5.63*(Y0FLAK/(XSNOW+1.E-20))**.3333
IF ((XSNOW.GE.1.E-12) .AND. (CLOUD.GT.0.)) THEN
  A0LAMB = 350.E-6*SLAMBD
  RIM = 0.319*Y0FLAK*(SLAMBD**-3.206)*EXP(-A0LAMB)*
      2 (A0LAMB*(A0LAMB+2.)+2.)
END IF
C

```

TABLE 5-8 Continued

```

C   FOR TEMPC < 0, CALCULATE
C   DEPOSITIONAL GROWTH RATE = DEPOSI
C   SUBLIMATION RATE = SUBLIM*SNOW
C   FREEZING RATE = FREEZ*RAIN
C
C   IN CALCULATIONS FOR THE SMALL, MONODISPERSE ICE-CRYSTAL CASE
C   YCRYST = CRYSTAL CONCENTRATION (NO/M**3)
C   XCRYST = INDIVIDUAL CRYSTAL MASS (GM)
C   DEPCRY = DEPOSITIONAL GROWTH RATE FOR THE CRYSTALS
C
C   IF (TEMPC .LT. 0.) THEN
C     YCRYST = AMAX1(0.006, 400.*((-TEMPC/16.)**4.))
C     XCRYST = AMAX1(XSNOW/YCRYST, 6.0E-11)
C     DIFH2O = 0.226E-4*((TEMP/273.15)**1.81)*(1.E6/PRESS(I))
C     GSI = 0.82*DIFH2O*(XVAPOR-VSATI*1.8E7)
C     DEPCRY = YCRYST*(0.196*XCRYST**0.38)*GSI*(1.+65.*XCRYST**.39)
C     IF (XSNOW .GE. 1.E-12) THEN
C       A0LAMB = AMAX1(0.,ALOG(Y0FLAK/(SLAMBD*YCRYST)))
C       YTFLAK = (Y0FLAK/SLAMBD)*EXP(-A0LAMB)
C       AFLAKE = (1.+A0LAMB)/SLAMBD
C       DEPOSI = YTFLAK*(6.28*AFLAKE)*GSI*(1.+374.*AFLAKE**0.75)
C     END IF
C     DEPOSI = AMAX1(DEPOSI,DEPCRY)/1.8E7
C     IF (DEPOSI .LT. 0.) THEN
C       SUBLIM = -DEPOSI/SNOW
C       SUBLIM = AMIN1( 1.0, SUBLIM )
C       DEPOSI = 0.
C     END IF
C
C     FREEZ = 2.57E-5*YCRYST*(XRAIN**0.63)
C     FREEZ = AMIN1( 1.0, FREEZ )
C
C   ELSE
C
C   FOR TEMPC > 0, CALCULATE
C   MELTING RATE = SMEL*SNOW
C   ALSO, RIM RATE TRANSFERS CLOUD WATER TO RAIN CATEGORY
C   RATHER THAN TO SNOW IN THIS CASE
C
C     RMELT = (TEMPC - 4.677E7*(2.693E-7-VAPOR))*
C   +       (7.492E-6*(SNOW**.667) + 7.415E-4*(SNOW**.868))
C   +       + 1.226E-2*TEMPC*RIM*CLOUD
C     SMEL = RMELT/AMAX1(SNOW, 1.E-25)
C     IF (SMEL .LT. 0.) SMEL = 0.
C     SMEL = AMIN1( 1.0, SMEL )
C     ACCR = ACCR + RIM
C     RIM = 0.
C   END IF

```

TABLE 5-8 Continued

```

C
C  CALC G TERMS FOR WATER SPECIES
C
      GGEN(KRAIN) = (AUTO+ACCR)*CLOUD + SMEL*SNOW
      GDEC(KRAIN) = (EVAP+FREEZ)*RAIN
      GGEN(KSNOW) = DEPOSI + RIM*CLOUD + FREEZ*RAIN
      GDEC(KSNOW) = (SMEL+SUBLIM)*SNOW
      GGEN(KVAPCL) = EVAP*RAIN + SUBLIM*SNOW
      GDEC(KVAPCL) = (AUTO+ACCR+RIM)*CLOUD + DEPOSI

C
C  LATENT HEATING TERMS
C      IF ISSAT(I) = 0, THEN TEMPERATURE ADV-DIFF EQUATION WAS INTEGRATED
C      UNSATURATED, SO CONSIDER ALL LATENT HEAT TERMS
C      OTHERWISE, TEMP. EQN. WAS INTEGRATED SATURATED, SO JUST CONSIDER
C      LATENT HEAT FROM WATER-ICE TRANSFORMATIONS, AND EVAPORATION
C
      IF (ITEMP.EQ. 0) GO TO 1000
      IF (ISSAT(I).EQ. 0) THEN
        DMCOND = DEPOSI - SUBLIM*SNOW - EVAP*RAIN
      ELSE
        DMCOND = -EVAP*RAIN
      END IF
      DMFREQ = DEPOSI - (SUBLIM+SMEL)*SNOW + RIM*CLOUD + FREEZ*RAIN
      GGEN(KTEMP) = (4.503E11*DMCOND + 5.2E10*DMFREQ)/CPCSPS(I)

1000  CONTINUE

C-----
C
C  COMPUTE CONSTRAINED VARIABLES
C-----
C      DK0H22 = H2O2 SOLUBILITY
C      PATM = PRESSURE IN ATMOSPHERES
C      HEXC = H+ CONC. IN CLOUD WATER (MOLAR)
C      SO2MF = SO2 EXPRESSED AS MASS FRACTION
C      HPRIME = "EFFECTIVE" SO2 SOLUBILITY
C
      CNN(KHIONR) = 2.53E-7*RAIN + 1.864*CNN(KSO4R)

      DK0H22 = 8.2414E-6*EXP(6834.93/TEMP)*82.0564*TEMP
      PATM = PRESS(I)/1.013E6
      CNN(KHIONC) = 2.53E-7*CLOUD + 1.864*CNN(KSO4C)
      IF (CLOUD.GE. CMIN(KCLOUD)) THEN
        HEXC = CNN(KHIONC)/(.018*CLOUD)
        SO2MF = CNN(KSO2GC)/CS(I)

```

TABLE 5-8 Continued

```

CALL HENRY( HPRIME, SO2MF, HEXC, TEMP, PATM, 0 )
XICS02 = 18.*CLOUD/(CS(I)*HPRIME)
CNN(KS02G) = CNN(KS02GC)/(1.+XICS02)
CNN(KS02C) = CNN(KS02GC) - CNN(KS02G)

XICH202 = .018*CLOUD*DK0H22
CNN(KH202G) = CNN(KH202GC)/(1.+XICH202)
CNN(KH202C) = CNN(KH202GC) - CNN(KH202G)
ELSE
  CNN(KS02G) = CNN(KS02GC)
  CNN(KS02C) = 0.
  CNN(KH202G) = CNN(KH202GC)
  CNN(KH202C) = 0.
ENDIF

IF (IGCALC .LE. 0) GOTO 8000

```

```

C-----
C
C  CALCULATE GENERATION AND DECAY RATES FOR POLLUTANT SPECIES
C
C-----

```

```

C
C  AEROSOL SCAVENGING
C
C  XNS04A = NO. OF SULFATE PARTICLES PER CM**3
C  ASCS04 = NUCLEATION RATE (MOLE/CC/SEC)
C
C  XNS04A = CNN(KS04A)/(.0053*(DPS**3))
C  IF (XNC .LT. XNS04A) THEN
C    FRACNU = XNC/XNS04A
C  ELSE
C    FRACNU = 1.
C  END IF
C  ASCS04 = CNN(KS04A)*FRACNU*(AUTO+ACCR+RIM)

```

```

C
C  FOLLOWING 8 VARIABLES HAVE UNITS OF MOLE/CC/SEC
C
C  XTDH202 = 0.      ! MASS TRANSFER OF H2O2 TO RAIN
C  XFDH202 = 0.      ! MASS TRANSFER OF H2O2 FROM RAIN
C  XTDSO2 = 0.       ! MASS TRANSFER OF SO2 TO RAIN
C  XFDSO2 = 0.       ! MASS TRANSFER OF SO2 FROM RAIN
C
C  SOXCH2 = 0.       ! REACTION OF SO2 AND H2O2 IN CLOUD
C  SOXRH2 = 0.       ! REACTION OF SO2 AND H2O2 IN RAIN
C  SOXCO2 = 0.       ! REACTION OF SO2 AND OZONE IN CLOUD
C  SOXRO2 = 0.       ! REACTION OF SO2 AND OZONE IN RAIN

```

TABLE 5-8 Continued

DK1S = EXP(-10.96+1970./TEMP)
! FIRST DISSOC. CONSTANT FOR AQUEOUS SO2

```

C
C  PROCESSES IN RAIN
C
      IF (RAIN .GT. 1.E-6/1.8E7 ) THEN
C.....SOLUBILITIES
          HEXR = CNN(KHIONR)/(.018*RAIN)      ! H+ CONC. IN RAIN (MOLAR)
          SO2MF = CNN(KSO2G)/CS(I)
          CALL HENRY( HPRIME, SO2MF, HEXR, TEMP, PATM, 0 )
          XIRS02 = 18.*RAIN/(CS(I)*HPRIME)
          XIRH202 = .018*RAIN*DK0H22
C.....MASS TRANSFER
          XFRATE = MASS TRANSFER RATE FROM LEVINE AND SCHWARTZ
          IF (JPASSO .EQ. 1) XFRATE = 31.2*(RAIN**.647)
          XTDS02 = XFRATE * CNN(KSO2G)
          XFDS02 = XFRATE * CNN(KSO2R)/XIRS02
          XTDH202 = XFRATE * CNN(KH202G)
          XFDH202 = XFRATE * CNN(KH202R)/XIRH202
C.....CHEMICAL REACTION
          SO2AQM = CONC. OF UNDISSOCIATED SO2 IN RAIN (MOLAR)
          SOXROZ = 2.9E6*CNN(KSO2R)*CNN(KO3G)/SQRT(HEXR)
          SO2AQM = (CNN(KSO2R)/(.018*RAIN))/
+                 (1. + (DK1S/HEXR))
          SOXRH2 = 8.3E5*SO2AQM*CNN(KH202R)

      ENDIF

```

```

C
C  PROCESSES IN CLOUD WATER
C
      IF (CNN(KCLOUD) .GT. CMIN(KCLOUD)) THEN
          SOXCOZ = 2.9E6*CNN(KSO2C)*CNN(KO3G)/SQRT(HEXC)
          SO2AQM = (CNN(KSO2C)/(.018*CLOUD))/
+                 (1. + (DK1S/HEXC))
          SOXCH2 = 8.3E5*SO2AQM*CNN(KH202C)
      ENDIF

```

```

C
C
C  COMPUTE GENERATION AND DECAY RATES
C
C

```

```

C...SO2
      GGEN(KSO2GC) = XFDS02 + SUBLIM*CNN(KSO2S)
      GDEC(KSO2GC) = (AUTO+ACCR+RIM)*CNN(KSO2C)
+      + SOXCH2 + SOXCOZ + XTDS02

```

TABLE 5-8 Continued

GGEN(KS02R) = (AUTO+ACCR)*CNN(KS02C) + SMEL*CNN(KS02S)
 + XTDS02
 GDEC(KS02R) = FREEZ*CNN(KS02R)
 + SOXRH2 + SOXROZ + XFDS02

GGEN(KS02S) = RIM*CNN(KS02C) + FREEZ*CNN(KS02R)
 GDEC(KS02S) = (SMEL+SUBLIM)*CNN(KS02S)

C...S04

GGEN(KS04A) = EVAP*CNN(KS04R) + SUBLIM*CNN(KS04S)
 GDEC(KS04A) = ASCS04

GGEN(KS04C) = ASCS04 + SOXCH2 + SOXCOZ
 GDEC(KS04C) = (AUTO+ACCR+RIM)*CNN(KS04C)

GGEN(KS04R) = (AUTO+ACCR)*CNN(KS04C) + SMEL*CNN(KS04S)
 + SOXRH2 + SOXROZ
 GDEC(KS04R) = (EVAP+FREEZ)*CNN(KS04R)

GGEN(KS04S) = RIM*CNN(KS04C) + FREEZ*CNN(KS04R)
 GDEC(KS04S) = (SMEL+SUBLIM)*CNN(KS04S)

C...H202

GGEN(KH202GC) = XFDH202 + SUBLIM*CNN(KH202S)
 GDEC(KH202GC) = (AUTO+ACCR+RIM)*CNN(KH202C)
 + XTDH202 + SOXCH2

GGEN(KH202R) = (AUTO+ACCR)*CNN(KH202C) + SMEL*CNN(H202S)
 + XTDH202
 GDEC(KH202R) = FREEZ*CNN(KH202R) + SOXRH2 + XFDH202

GGEN(KH202S) = RIM*CNN(KH202C) + FREEZ*CNN(H202R)
 GDEC(KH202S) = (SMEL+SUBLIM)*CNN(KH202S)

C...OZONE

GDEC(K03G) = SOXCOZ + SOXROZ

8000 CONTINUE
 RETURN
 END

discussed earlier in part B. The Class III subroutine HENRY is used to compute the H' of Equation (69), which is needed for the SO_2 equilibrium. The equilibria for aqueous O_3 ,

are computed later, since the aqueous O_3 concentrations are just used as temporary variables, unlike the aqueous SO_2 and H_2O_2 variables. Again, this is possible because O_3 has a very low solubility; thus the aqueous O_3 concentrations are very small compared to the corresponding gas concentrations.

The next section computes rates for the following processes: nucleation scavenging, mass transfer between gas and rainborne species, and chemical reaction of aqueous species. Note that the mass transfer to rain and the aqueous reactions in rain are "enabled" only when the rain concentration is above 10^{-6} gm/m^3 . This artificial cutoff has been inserted to improve computational efficiency. The justification is that the impact of these processes is negligible when the amount of rain is below the cutoff value. One should note also that in the mass-transfer section, the variable XFRATE which is Λ in Equation (73) is only computed on the predictor pass (JPASSO = 1). This approximation has little effect when rain concentrations are significant, but improves computational speed at low rain concentrations.

Finally, the net generation and decay rates are computed for each species. It is worthwhile to work through this section of the code using Figures 5-2 and 5-3. Note that most terms occur in one species generation expression and in one species decay expression. The exceptions are chemical reaction terms which involve two reactants: these terms thus occur in two decay expressions.

SUBROUTINE GRDSET (Table 4-8)

GRDSET establishes the vertical spacing of the computational grid. For this example, uniform spacing is again used, so GRDSET is the same as the Example 1 version.

SUBROUTINE SETTLE (Table 5-9)

SETTLE establishes the settling velocities of the computed species. In this example, rain, snow, and any precipitation-borne species have significant settling velocities. These velocities are the mass-weighted mean velocities for the rain and snow Marshall-Palmer size distributions, and are computed as described in the first part of this chapter. As these velocities are concentration dependent and change with time, we need ISETTLE = 1.

SUBROUTINE TIMESP (Table 5-10)

TIMESP sets the basic integration time step, DT. In this example, precipitation species can have significant settling velocities (approaching 10^3 cm/sec), and computational constraints require that DT not be too large. In particular, it is important to keep the local Courant number near or below unity. This requires that

$$DT \cdot URATIO \cdot W \leq DZ$$

at all grids, where W is the largest of the vertical velocities and DZ is the local grid spacing. In this example, we have also set an upper limit for DT of 60 secs.

SUBROUTINE USHEAR (Table 5-11)

USHEAR establishes the ratio $URATIO = u^*/u_A$. This example is a two-dimensional time-dependent simulation, with u_A varying in height. In particular, u_A varies linearly from 5 m/sec at $z = 0$ to 10 m/sec at $z = 1.5$ km, and is constant at 10 m/sec above this height. The reference level has been chosen as the grid top, so $u^* = 10$ m/sec. The horizontal wind speed is constant in time for the example, so USHEAR only needs to be called initially and ISHEAR = 0.

TABLE 5-9. Listing of Subroutine SETTL for Example Application 2

```

SUBROUTINE SETTL (INIT)
C
C   SETTL COMPUTES SETTLING VELOCITIES FOR EACH SPECIES
C   FOR THIS EXAMPLE, ONLY RAIN AND SNOWBORNE SPECIES HAVE
C   NON-ZERO SETTLING VELOCITIES
C
C   INCLUDE 'PLUVCMN'
C
C   ON INITIAL ENTRY, ZERO SETTLING VELOCITIES
C
C   IF (INIT .EQ. 1) THEN
C       DO I = 1, N
C           DO K = 1, NCOMP
C               WR(I,K) = 0.0
C           END DO
C       END DO
C   END IF
C
C   DO I = 1,N
C
C   CALCULATE RAIN SETTLING VELOCITY
C       XRAIN = CONC. IN GM/M**3
C       RLAMBD = LAMBDA OF MARSHALL-PALMER DISTRIBUTION
C
C       XRAIN = AMAX1(C(I,KRAIN)*1.8E7, 1.E-10)
C       RLAMBD = 2367.*(XRAIN)**(-.25)
C       A0L = 1.02E-3*RLAMBD
C       EA0L = EXP(-A0L)
C       FACT3 = 1.+A0L*(1.+(A0L/2.)*(1.+A0L/3.))
C       FACT4 = 1.-EA0L*(FACT3 + (A0L**4.)/24.)
C       FACT3 = 1.-EA0L*FACT3
C       FACT34 = SQRT(FACT3*FACT4)
C       VBAR = (1.-FACT34)*1.94*130./SQRT(RLAMBD) +
+       FACT4*4.*4055./RLAMBD
C       VRain = -VBAR/1.0E-2
C
C       WR(I,KRAIN) = VRain
C       WR(I,KSO4R) = VRain
C       WR(I,KSO2R) = VRain
C       WR(I,KH2O2R) = VRain
C
C   CALCULATE SNOW SETTLING VELOCITY
C       XSNOW = CONC. IN GM/M**3
C       SLAMBD = LAMBDA OF MARSHALL-PALMER DISTRIBUTION

```

TABLE 5-9 Continued

```

C      YØFLAK = NØ,S OF MARSHALL-PALMER DISTRIBUTION
C
      XSNOW = AMAX1(Ø., C(I,KSNOW)*1.8E7)
      TEMPC = C(I,1)-273.15
      YØFLAK = 5.681E6*EXP(-Ø.Ø878*AMIN1(TEMPC,Ø.))
      SLAMBD = 5.63*(YØFLAK/(XSNOW+1.E-2Ø))**Ø.3333
      AFLAKE = 1./SLAMBD
      VBARG = 3.33*(AFLAKE**.2Ø6)*1.22
      IF (AFLAKE.LT.3.37E-4) VBARG = 473.Ø*(AFLAKE**.927)*2.74
      VSNOW = -VBARG/1.ØE-2

      WR(I,KSNOW) = VSNOW
      WR(I,KSO4S) = VSNOW
      WR(I,KSO2S) = VSNOW
      WR(I,KH2O2S) = VSNOW

      END DO

      RETURN
      END

```

TABLE 5-10. Listing of Subroutine TIMESP for Example Application 2

```

SUBROUTINE TIMESP
C
C TIMESP SETS ADVECTION-DIFFUSION INTEGRATION TIME STEP
C THIS VERSION MAINTAINS THE COURANT NUMBER ( $w \cdot DTEFF/DZ$ ) AT OR
C BELOW THE VALUE "COURMX", AND THE TIME STEP BELOW DTMX
C (DTEFF = EFFECTIVE TIME STEP =  $DT \cdot URATIO$ )
C
      INCLUDE 'PLUVCMN'
      DATA COURMX, DTMX /.9, 60./

      DNEW = 1.E10
      DO 30 I = 1,N
        J = MAX0(I, 2)
        DZSTAR = Z(J) - Z(J-1)
        WMAX = AMAX1( 1.E-10, ABS(WAP(I)), ABS(WAP(I)+WR(I,KRAIN)),
+          ABS(WAP(I)+WR(I,KSNOV)) )
        DTADV = DZSTAR/(WMAX*URATIO(I))
        DNEW = AMIN1( DNEW, DTADV )
30    CONTINUE
      DT = AMIN1(DNEW*COURMX,DTMX)

      RETURN
      END

```

TABLE 5-11. Listing of Subroutine USHEAR for Example Application 2

```

SUBROUTINE USHEAR(INIT)
C
C USHEAR COMPUTES URATIO(I) = UA(IREF)/UA(I)
C   WHERE UA IS THE HORIZONTAL WIND SPEED AT HEIGHT Z(I) AND
C   IREF IS A SPECIFIED REFERENCE LEVEL (FIXED FOR THE MODEL RUN)
C   FOR ONE-DIMENSIONAL TIME-DEPENDENT SIMULATIONS WITH NO SHEAR,
C   SET URATIO(I) = 1. FOR ALL I.
C
C   INCLUDE 'PLUVCMN'
C
C   FOR THIS EXAMPLE, WIND INCREASES LINEARLY FROM 500 CM/S AT SURFACE
C   TO 1000 CM/S AT 1.5 KM, AND IS CONSTANT (1000 CM/S) ABOVE.
C   REFERENCE LEVEL IS AT GRID TOP
C
  USTAR = 10.E2
  DO I = 1,N
    IF (Z(I) .GT. 1.5E5) THEN
      UA = 10.E2
    ELSE
      UA = 5.E2 + 5.E2*(Z(I)/1.5E5)
    END IF
    URATIO(I) = USTAR/UA
  END DO

  RETURN
END

```

SUBROUTINE VERT (Table 5-12)

VERT establishes the two components of the air vertical velocity as given in Equation (11). For this example, the component relative to the grid, w_A'' , has been arbitrarily specified as zero. The other component, the grid vertical velocity, is determined by the shape of the hypothetical orographic barrier shown in Figure 5-1. At the bottom grid level, this velocity is given by

$$w_{Ao} = u_A \frac{dz_G}{dx}$$

where z_G is the height of the barrier. The time and distance coordinates are related by $x = u^*t^*$, so that

$$w_{Ao} = \frac{u_A}{u^*} \frac{dz_G}{dt^*}$$

The ground profile and the resulting dz_G/dt , is the arbitrarily chosen mathematical function shown in Figure 5-1. As noted in the USHEAR discussion of Chapter 3, the PLUVIUS array WAGRID is defined by

$$WAGRID(1) \equiv w_{Ao}$$

$$\text{and } WAGRID(I) \equiv w_{Ao} (u_A/u_{Ao}) = WAGRID(1)*URATIO(1)/URATIO(I) \quad .$$

E. CLASS III SUBROUTINE DESCRIPTIONS

Two Class III subroutines are used in this example. Both are called by subroutine GEN.

Subroutine HENRY (Table 5-13) computes the effective solubility parameter for SO_2 , as described in Equations (68)-(71). The subroutine was borrowed directly from a previous code (Drewes and Hales, 1977).

FUNCTION SSAT (Table 5-14) computes the saturation vapor density with respect to ice, and is needed to calculate the depositional growth rate for snow.

TABLE 5-12. Listing of Subroutine VERT for Example Application 2

```

SUBROUTINE VERT
  INCLUDE 'PLUVCMN'

  PARAMETER (PI = 3.1415927)

C
C  PARAMETERS DEFINING THE HYPOTHETICAL GROUND PROFILE:
C  UPSLOPE REGION IS FROM TW1 TO TW2, DOWNSLOPE IS FROM TW3 TO TW4.
C  ZGMAX IS MAXIMUM HEIGHT OF THE GROUND PROFILE.
C  DZGDT IS RATE OF CHANGE OF GROUND HEIGHT (ZG) WITH TIME
C

  PARAMETER (TW1=900., TW2=4500., TW3=8100., TW4=11700.)
  PARAMETER (ZGMAX = 1.E5)

  IF ((TCLOCK.GT.TW1) .AND. (TCLOCK.LT.TW2)) THEN
    DZGDT = (0.5*PI*ZGMAX/(TW2-TW1)) *
+     SIN( PI*(TCLOCK-TW1)/(TW2-TW1) )
  ELSE IF ((TCLOCK.GT.TW3) .AND. (TCLOCK.LT.TW4)) THEN
    DZGDT = -(0.5*PI*ZGMAX/(TW4-TW3)) *
+     SIN( PI*(TCLOCK-TW3)/(TW4-TW3) )
  ELSE
    DZGDT = 0.
  ENDIF
  WAGRID1 = DZGDT/URATIO(1)

  DO I = 1,N
    WAP(I) = 0.
    WAGRID(I) = WAGRID1*URATIO(1)/URATIO(I)
  END DO

  RETURN
END

```


TABLE 5-13. Listing of Subroutine HENRY for Example Application 2

```

SUBROUTINE HENRY ( HPRIME, C, HEX, T, P, LGOPT )
C
C SUBROUTINE FOR CALCULATING APPARENT HENRY'S LAW CONSTANT
C ON THE BASIS OF JOHNSTONE-LEPPLA PARAMETERS
C HPRIME IS THE APPARENT HENRY'S LAW CONSTANT, DEFINED BY:
C  $HPRIME = SO2\text{-}GAS / SO2\text{-}AQ$ , WHERE:
C  $SO2\text{-}AQ$  = CONCENTRATION OF SULFUR-IV IN AQUEOUS PHASE
C (MOLES/CM**3 WATER)
C  $SO2\text{-}GAS$  = CONCENTRATION OF GAS PHASE SO2 (MOLE FRACTION)
C C IS EITHER
C  $SO2\text{-}AQ$  WHEN LGOPT = 1 (MOLES/CM**3 WATER)
C  $SO2\text{-}GAS$  WHEN LGOPT = 0 (MOLE FRACTION)
C HEX IS THE AQUEOUS PHASE HYDROGEN ION CONCENTRATION FROM SPECIES
C OTHER THAN SULFUR-IV (MOLAR)
C T IS TEMPERATURE (DEGREES K)
C P IS ATMOSPHERIC PRESSURE (ATMOSPHERES)
C LGOPT IS A FLAG EXPLAINED ABOVE
C

IF ((LGOPT.NE.0) .AND. (LGOPT.NE.1)) STOP 7777
HANK = EXP(10.21-3112./T)/P
EQCON = EXP(-10.96+1970./T)
B = EQCON+HEX

C
C LGOPT=1 --> C IS THE AQUEOUS CONCENTRATION
C
IF (LGOPT .NE. 1) GOTO 20
CDUM = EQCON*1000.*C
TEST1 = 4.*CDUM/(B*B)
IF (TEST1 .GT. .001) GOTO 10
C.....LOW CONCENTRATIONS - USE ASYMPTOTIC EXPRESSION
HPRIME = HANK*(1.-EQCON/B)
GOTO 40
C.....SOLVE TOTAL SOLUBILITY EQUATION
10 HPRIME = HANK*(1.+(B-SQRT(B*B+4.*CDUM))/(2000.*C))
GOTO 40

C
C LGOPT=0 --> C IS THE GAS PHASE CONCENTRATION
C
20 TEST1 = 4.*EQCON*C/(HEX*HEX*HANK)
IF (TEST1 .GT. .001) GOTO 30
C.....LOW CONCENTRATIONS - USE ASYMPTOTIC EXPRESSION
HPRIME = HANK*HEX/B
GOTO 40

```

TABLE 5-13 Continued

```
C.....SOLVE TOTAL SOLUBILITY EQUATION
30      HPRIME = C/(C/HANK-(HEX-SQRT(HEX*HEX+4.*C*EQCON/HANK))/2.)

40      HPRIME = HPRIME*1000.
      RETURN
      END
```

TABLE 5-14. Listing of Function SSAT for Example Application 2

FUNCTION SSAT (TEMPK)

C
C
C
C
C

SSAT = THE SATURATION CONCENTRATION OF WATER VAPOR (GRAM MOLES/CC)
OVER ICE AT TEMPK DEGREES KELVIN
(ESAT IS SATURATION VAPOR PRESSURE IN MB)

TEMPC = TEMPK - 273.15

ESAT = 6.109177956 + TEMPC*(5.034698970E-1 + TEMPC*(1.886013408E-2
+ TEMPC*(4.176223716E-4 + TEMPC*(5.824720280E-6

+ TEMPC*(4.838803174E-8 + TEMPC*(1.838826904E-10))))))

SSAT=(ESAT*1.E3)/(8.3144E7*TEMPC)

RETURN

END

F. MODEL OUTPUT

Printed output from Example Application 2 is reproduced in the tables of Appendix D. Some of the more interesting features of the simulation are shown in Figures 5-4 through 5-6.

Figure 5-4 shows the time-height distributions of cloud water, rain, and snow (which were shown schematically in Figure 5-1). These should be viewed as two-dimensional, x-z distributions. A cloud forms on the upwind side of the orographic barrier, then dissipates on the downwind side. Initially, snow growth is most rapid at higher elevations because of the temperature dependence of deposition growth. The highest snow concentrations are at lower elevations, however, because the "concentration" represents the cumulative growth as snow particles descend. The melting level at about 2.5 km is quite apparent. Note that rain concentrations beneath the melting level are lower than the snow concentration above it, because rain has a higher fallspeed than snow and it is the precipitation flux that is conserved across the layer.

Figure 5-5 shows time-height distributions for SO_2 , sulfate, and H_2O_2 . Note that the total concentration (i.e., the sum of gaseous/aerosol, cloud water, rain, and snow phases) of each species is shown. Ozone is only slightly depleted by scavenging so has not been shown. The H_2O_2 distribution is the easiest to interpret: essentially all H_2O_2 is destroyed by the aqueous reaction with SO_2 shortly after the cloud forms. The SO_2 distribution shows the effects of moderate depletion by aqueous reaction and non-reactive scavenging, and a broadening of the initial sharp vertical concentration gradient by diffusion. The H_2O_2 reaction accounts for a 10% SO_2 loss. (Initial $\text{H}_2\text{O}_2/\text{SO}_2$ ratio is 0.1.) The total SO_2 loss is somewhat greater than 20% at higher elevations (initial 2 ppb, final <1.6 ppb), and somewhere between 10 and 20% at lower elevations. This is explained by the inverse dependences of both the SO_2 -ozone reaction and SO_2 solubility on H^+ concentration. The H^+ concentration is highest at low elevations where there is more sulfate. The sulfate distribution is interesting in that it shows the competing effects of production (by aqueous reaction of SO_2) and loss (by precipitation scavenging). This results in a peak concentration of 2 ppb at about 1 hour into the

FIGURE 5-4. Distributions of Cloud Water, Rain, and Snow in Example Application 2. Contour units are gm/m^3 . A time of 1 hour corresponds to a horizontal distance of 36 km.

FIGURE 5-5. Distributions of Total SO₂, Total SO₄, and Total H₂O₂ Mixing Ratios in Example Application 2. The "total" is the sum of the species in gas/aerosol, cloud, rain, and snow forms. Contour units are ppb. A time of 1 hour corresponds to a horizontal distance of 36 km.

FIGURE 5-6. Rain Rate (J), Concentrations of Rainborne Pollutant (CONC), and Deposition Rates of Rainborne Pollutant (DEP) at the Surface (i.e., the bottom grid element) in Example Application 2. Dotted line in top subplot is the height of the orographic barrier. A time of 1 hour corresponds to a horizontal distance of 36 km.

simulation. At higher elevations, the final concentration is greater than the initial concentration, indicating that the production is greater than the loss in this region.

Figure 5-6 shows the surface rainfall rate, rainborne pollutant concentrations, and rainborne pollutant deposition rates. The rainfall rate shows an initial peak corresponding to the one in Figure 5-4, then a secondary peak about a half-hour later. Fluctuations like this are a result of the nonlinear nature of the precipitation growth and fallspeed parameterizations. The sulfate concentration decreases monotonically-- showing the gradual depletion of primary and secondary sulfate by scavenging. The H^+ concentration follows the sulfate concentration, as constrained by Equation (72). The SO_2 concentration increases with time, because of the inverse relation between its solubility and H^+ concentration. The relative contributions of primary (aerosol) sulfate and secondary sulfate to the surface deposition cannot be ascertained from this single simulation. However, one could simply run a second simulation in which the initial SO_2 concentration is everywhere zero to obtain the primary sulfate deposition.

6. PROBLEMS WITH PLUVIUS: SOME PRACTICAL DIFFICULTIES AND SUGGESTIONS FOR THEIR RESOLUTION

Aside from the inherent one-dimensionality of PLUVIUS, there are a number of practical difficulties which can emerge with the model to produce malfunctions or inappropriate results, and several actions can be taken to minimize these effects. The first and most important of these is simply the problem of formulating a conceptual model and implementing it on PLUVIUS in a correct and expedient fashion. There is no easy solution to this; but our experience has shown that significant shakedown and backtracking time can be eliminated via systematic use of a formal implementation procedure. The procedure is as follows:

- Create interaction diagrams (e.g., Figures 5-2 and 5-3) to define all pathways and dependent variables.
- Create a species-definition table (eg. Table 5-1) to define specifically the interactive species within the computation.
- Create a table of initial conditions.
- Determine the number of diffusion regimes.
- Adjust the code's dimensioning to be sufficiently large to accommodate these parameters.
- Ensure that the water-related variables (if employed) are named in a manner that is consistent with usage in the main program (cf. Section 3A).
- Define all required boundary conditions.
- Define grid height and temporal and spatial spacing.
- Define vertical movement of grid and relative vertical flows (w_A').
- Define fall-velocity features.
- Define diffusional behavior.

the Class I subroutines to conform with the above specifications. A check-off list for this purpose is as follows:

ADJUST
BOUND
DIFF
GEN
GRDSET
SETTL
SETUP
TIMESP
USHEAR
VERT

consolidate the above subroutines with PLUVIUS and the Class II subroutines.

Add any required Class III subroutines.

Create an input data set as described in Section 3C (e.g., Table 5-2).

Execute the program.

second problem with PLUVIUS, which may arise to plague the user, is in the ordinary differential equation integration routine ODEINT. This routine was chosen for present purposes because of its low start-up "leads" and its generally efficient integration of stiff sets of equations. It is potentially susceptible to problems in two areas, however:

1. Integration of locally nonlinear systems: In general ODEINT requires rather small step sizes to integrate equations of the form

$$\frac{dA}{dt} = -kA^{\alpha} \quad \alpha \neq 1$$

This is not a major problem, except that it sometimes detracts rather substantially from the code's efficiency. Most chemical-

kinetics equations do not follow the above form. However, several cloud-physics parameterizations do involve nonlinear expressions of this type and thus tend to slow the code's execution rate.

2. Integration of some interactive systems: Typically ODEINT performs well in integrating complex multicomponent systems, such as air-chemistry schemes. There are, however, some exceptions which arise whenever specific reaction patterns occur; for example, the scheme

often can be integrated incorrectly by ODEINT, simply because some relatively significant terms can be overshadowed by others. Because of this, the user is well-advised to test ODEINT performance against more conventional simulations of his system (at only a single grid point), before embarking on extensive production runs. The user can, of course, replace ODEINT with a more trustworthy integration scheme, such as a Gear-based algorithm (Gear, 1971). Typically, however, such schemes demand large amounts of computer time for start-up overheads, thus reducing their appeal rather substantially.

Returning to the question of one-dimensionality, it should be noted that although this is a major shortcoming of PLUVIUS, its effects can be minimized by appropriate applications within the code. Three-dimensional plumes, for example, may be simulated by diluting the air parcel to account for cross-plume mixing by providing time-dependent dilution factors within subroutine GEN. Three-dimensional flow fields can be approximated in a

similar manner, with judicious choice of the vertical-velocity component w_A , (a)

In a final analysis, it is once again noted that PLUVIUS embodies a somewhat gross approximation to the real world, and constitutes a rather imperfect "lens" through which to observe atmospheric behavior. With this qualification, however, it is expected that prudent application of the code can lead to a number of revealing and scientifically rewarding insights. It is with this intent that PLUVIUS is submitted to the user community.

(a) It should be noted that the problem of one-dimensionality has been solved with the newer "PLUVIUS II" code, which allows computations in 1, 2, or 3 spatial dimensions at the option of the user. Currently operational, it is expected that PLUVIUS II will be documented in a future user's manual.

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APPENDIX A

FINITE DIFFERENCE APPROXIMATION FOR TRANSPORT TERMS

In this appendix, the finite differencing procedure employed in PLUVIUS Mod 5 to integrate the transport terms (advection and diffusion) of the mass- and energy-balance equations is described. The method uses Crank-Nicholson time-differencing and a combination of spatial-differencing techniques. Centered differencing for the diffusion terms and "compact" spatial-differencing for the advection terms (Adams, 1975 and 1977). This combination was adopted because the compact differencing method for both the advection and diffusion terms showed poor performance on some test problems (e.g., a single grid point "inversion," where the eddy diffusivity was set to zero). The method adopted is unconditionally stable (for linear problems). The time-differencing and centered spatial-differencing have second-order truncation errors, and the compact spatial-differencing has a fourth-order truncation error (for uniform grids).

The numerical problem is the integration of Equations (42) and (44) (or the corresponding two-dimensional, steady-state equations) over a time step Δt from time t_j to t_{j+1} , where the values of c are known only at the discrete grid points $z_1, z_2, \dots, z_n$. In general, the various coefficients in the equations (w_r, w_A, D, c^* , etc.) will be functions of time and space. They may also be functions of c , the dependent variable, thus making the equations nonlinear. In the development here, the dependence of these coefficients on time and on the dependent variable c is assumed negligible over the time step Δt and is ignored.

In the following development, c_i^j will be used to denote c at time t_j and vertical position z_i , and similarly for other variables. The superscript j will be dropped on terms where the variation over Δt is ignored (e.g., w_A, c^*, D), as it will always be j and not $j+1$ in these cases. Time derivatives are indicated by the subscript t ($c_t = \hat{D}c/\hat{D}t$ or D^*c/Dt^*) and spatial derivatives by the subscript z or ξ ($c_z \equiv \partial c/\partial z$).

The differencing procedure will be developed for the mass-balance equation for the two-dimensional, steady-state case:

$$\frac{D^*c}{Dt^*} = \mu \left\{ - \frac{\partial}{\partial z} \left[(w_r + w_A'')c \right] + \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right] + c \frac{\partial w_A''}{\partial z} + c \frac{w_A}{c^*} \frac{\partial c^*}{\partial z} + D1 \right\} \quad (A1)$$

where $\mu = u^*/u_A^*$. The term D1 has been added in anticipation of the energy-balance equation; in the mass-balance equation $D1 \equiv 0$. The mass-balance equation for the one-dimensional time-dependent case is handled identically, but with $\mu \equiv 1$. The energy-balance equation involves some modifications which are discussed at the end of this appendix.

Crank-Nicholson time-differencing approximates the time derivative in Equation (A1) as follows:

$$\begin{aligned} (c_t)_i^{j+1/2} &\approx \frac{c_i^{j+1} - c_i^j}{\Delta t} \\ &= \frac{1}{2} \left\{ \left[\text{right-hand side of (A1)} \right]_i^{j+1} + \left[\text{right-hand side of (A1)} \right]_i^j \right\} \end{aligned} \quad (A2)$$

Before developing the "right-hand side of (A1)," which involves spatial differencing in several terms, we introduce a vertical coordinate transformation which will allow both uniform and non-uniform grid spacing to be treated alike. The new vertical coordinate, ξ , is just the vertical grid index

$$\xi \equiv i \quad \text{at} \quad z = z_i \quad .$$

Vertical derivatives are transformed as:

$$\frac{\partial c}{\partial z} = \frac{\partial \xi}{\partial z} \frac{\partial c}{\partial \xi} = \frac{1}{\Delta z} \frac{\partial c}{\partial \xi} \quad .$$

where

$$\Delta z \equiv \frac{\partial z}{\partial \xi}$$

At interior grid points, Δz is approximated using

$$\Delta z_i = \frac{1}{2} (z_{i+1} - z_{i-1}) \quad ,$$

and at the grid boundaries,

$$\Delta z_n = z_n - z_{n-1}$$

$$\Delta z_1 = z_2 - z_1 \quad .$$

Note that for uniform grids, these relations are exact.

To develop the advection term in Equation (A1), we define:

$$w_v = w_r + w_A''$$

$$R = \frac{\partial}{\partial \xi} (w_v c) \quad .$$

The advection term is then

$$\frac{\partial}{\partial z} \left[(w_r + w_A'') c \right] = \frac{R}{\Delta z} \quad . \quad (A3)$$

Evaluation of R involves a spatial derivative which is approximated using the compact differencing method (Adams, 1975 and 1977). At interior grids ($i = 2, 3, \dots, n-1$), the method yields:

$$R_{i-1}^j + 4R_i^j + R_{i+1}^j + 3(w_v c)_{i-1}^j - 3(w_v c)_{i+1}^j = 0 \quad . \quad (A4)$$

At the grid boundaries, the following relations hold:

$$R_1^j + R_2^j + 2 (w_v c)_1^j - 2 (w_v c)_2^j = 0 \quad (A5)$$

$$R_{n-1}^j + R_n^j + 2 (w_v c)_{n-1}^j - 2 (w_v c)_n^j = 0 \quad (A6)$$

Identical equations hold at t_{j+1} . At time t_j , Equations (A4)-(A6) form a set of n linear equations with n unknowns (R_i^j , $i = 1, 2, \dots, n$), since w_v and c are known. The equations are tri-diagonal in nature and can be solved using Thomas's algorithm. In the PLUVIUS code, this computation is performed in subroutines FIRSTD and TRIDAG.

The diffusion term in Equation (A1) is developed as follows. Define

$$Q_i^j = \left[D_m c^* \frac{\partial}{\partial z} \left(\frac{c}{c^*} \right) \right]_i^j \quad (A7)$$

Here the spatial derivative is approximated by a simple centered difference, and the Q 's are evaluated "between grid points", so that

$$Q_{i+1/2}^j = \frac{(D_m c^*)_{i+1/2}}{\Delta z_{i+1/2}} \left[\left(\frac{c}{c^*} \right)_{i+1}^j - \left(\frac{c}{c^*} \right)_i^j \right] \quad (A8)$$

where $\Delta z_{i+1/2} = z_{i+1} - z_i$. The diffusion term is then

$$\begin{aligned} \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} \left(\frac{c}{c^*} \right) \right]_i^j &= \frac{1}{\Delta z_i} \left(Q_{i+1/2}^j - Q_{i-1/2}^j \right) \\ &= A_{DIFF_i} c_{i-1}^j + B_{DIFF_i} c_i^j + C_{DIFF_i} c_{i+1}^j \end{aligned} \quad (A9)$$

where

$$\begin{aligned} A_{DIFF_i} &= \frac{1}{\Delta z_i c_{i-1}^*} \left(\frac{D_m c^*}{\Delta z} \right)_{i-1/2} \\ B_{DIFF_i} &= - \frac{1}{\Delta z_i c_i^*} \left[\left(\frac{D_m c^*}{\Delta z} \right)_{i+1/2} + \left(\frac{D_m c^*}{\Delta z} \right)_{i-1/2} \right] \end{aligned}$$

$$CDIFF_i = \frac{1}{\Delta z_i c^*_{i+1}} \left(\frac{D_m c^*}{\Delta z} \right)_{i+1/2}$$

The air density, c^* , is evaluated at $i+1/2$ by simply averaging the values at adjacent grid points. The eddy diffusivity, D_m , is defined between the grid points, at $z_{i+1/2}$, rather than at the grid points, z_i . The convention used is

$$D(I,L) \equiv (D_m)_{i+1/2}$$

where $D(I,L)$ is the two-dimensional array that holds the eddy diffusivities in PLUVIUS. (L specifies the diffusion regime, see Section 3.)

The third and fourth terms on the right-hand side of Equation (A1) involve spatial derivatives of w_A'' and c^* . We define

$$\begin{aligned} Cl_i &= \left(w_{Az}'' + \frac{w_A}{c^*} c_z^* \right)_i \\ &= \left[\frac{1}{\Delta z} \left(w_{A\xi}'' + \frac{w_A}{c^*} c_\xi^* \right) \right]_i \end{aligned} \quad (A10)$$

The derivatives $w_{A\xi}''$ and c_ξ^* are evaluated using the compact differencing technique, similar to the evaluation of R . For example, at interior grids, we have

$$c_{\xi i-1}^* + 4c_{\xi i}^* + c_{\xi i+1}^* + 3c_{i-1}^* - 3c_{i+1}^* = 0$$

In the PLUVIUS code, Cl is evaluated in subroutine DERIV, which makes calls to subroutine FIRSTD to evaluate the derivatives.

Equation (A2) can now be rewritten, at interior grid points, using Equations (A3), (A9), and (A10), as

$$\begin{aligned}
c_i^{j+1} - c_i^j = & -\frac{\epsilon}{\Delta z_i} \left(R_i^{j+1} + R_i^j \right) + \epsilon \left[\text{ADIFF}_i \left(c_{i-1}^{j+1} + c_{i-1}^j \right) \right. \\
& + \text{BDIFF}_i \left(c_i^{j+1} + c_i^j \right) + \left. \text{CDIFF}_i \left(c_{i+1}^{j+1} + c_{i+1}^j \right) \right] \\
& + \epsilon \text{Cl}_i \left(c_i^{j+1} + c_i^j \right) + 2\epsilon \text{Dl}_i
\end{aligned} \tag{A11}$$

where

$$\epsilon = \frac{1}{2} \mu \Delta t \quad .$$

Equations (A4) and (A11) may be combined to form

$$\text{AM}_i \text{XV}_{i-1}^{j+1} + \text{BM}_i \text{XV}_i^{j+1} + \text{CM}_i \text{XV}_{i+1}^{j+1} = \text{DV}_i \tag{A12}$$

Here XV_i^j represents a two-element vector,

$$\text{XV}_i^j = \begin{bmatrix} c_i^j \\ R_i^j \end{bmatrix} \quad ,$$

The AM, BM, and CM are each 2 x 2 matrices, and DV is a two-element vector:

$$\text{AM}_i = \begin{bmatrix} -\epsilon \text{ADIFF}_i & 0 \\ 3 w_{vi-1} & 1 \end{bmatrix} \tag{A13}$$

$$\text{BM}_i = \begin{bmatrix} 1 - \epsilon \text{BDIFF}_i - \epsilon \text{Cl}_i & \frac{\epsilon}{\Delta z_i} \\ 0 & 4 \end{bmatrix} \tag{A14}$$

$$\text{CM}_i = \begin{bmatrix} -\epsilon \text{CDIFF}_i & 0 \\ -3 w_{vi+1} & 1 \end{bmatrix} \tag{A15}$$

$$DV_i = \begin{bmatrix} c_i^j + \epsilon \left(ADIFF_i c_{i-1}^j + BDIFF_i c_i^j + CDIFF_i c_{i+1}^j \right. \\ \left. + Cl_i c_i^j + 2 D1_i - \frac{R_i^j}{\Delta z_i} \right) \\ 0 \end{bmatrix} \quad (A16)$$

Equation (A12) can be applied at all grid points. Equations (A13)-(A16) hold only at interior grid points. Different expressions for AM, BM, CM, and DV must be formulated at the grid boundaries for each set of boundary conditions [Equations (15)-(18) and (38)-(41)].

Concentration boundary conditions are the simplest to treat. At the top boundary, a concentration boundary condition gives

$$AM_n = \begin{bmatrix} 0 & 0 \\ 2w_{vn-1} & 1 \end{bmatrix} \quad (A17)$$

$$BM_n = \begin{bmatrix} 1 & 0 \\ -2w_{vn} & 1 \end{bmatrix} \quad (A18)$$

$$DV_n = \begin{bmatrix} \hat{c}_T^{j+1} \\ 0 \end{bmatrix} \quad (A19)$$

At the bottom boundary, a concentration boundary condition yields:

$$BM_1 = \begin{bmatrix} 1 & 0 \\ 2w_{v1} & 1 \end{bmatrix} \quad (A20)$$

$$CM_1 = \begin{bmatrix} 0 & 0 \\ -2w_{v2} & 1 \end{bmatrix} \quad (A21)$$

$$DV_1 = \begin{bmatrix} \hat{c}_B^{j+1} \\ 0 \end{bmatrix} \quad (A22)$$

Note that CM_n and AM_1 are "irrelevant" (since XV_0 and XV_{n+1} do not exist). Also, the bottom row elements in Equations (A17)-(A22) result from Equations (A5) and (A6).

The flux-specified boundary condition is more involved. Note that Equation (A11) could be applied at the grid-boundaries were it not for the diffusion term; thus an alternate treatment of this term is required at the boundaries. At the bottom boundary, the diffusion term is approximated by

$$\frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right]_1^j = \frac{1}{\left(\frac{\Delta z_1}{2} \right)} (Q_{3/2}^j - Q_1^j) \quad (A23)$$

The term $Q_{3/2}^j$ is evaluated as in Equation (A8). For Q_1^j , we can use the flux boundary condition [Equation (18)] to write

$$Q_1^j = (w_r c)_1^j - \hat{f}_B^j \quad (A24)$$

Thus the diffusion term can be written as

$$BDIFF_1 c_1^j + CDIFF_1 c_2^j - \frac{2}{\Delta z_1} (w_r c)_1^j + \frac{2}{\Delta z_1} \hat{f}_B^j \quad (A25)$$

where

$$BDIFF_1 = - \frac{2}{\Delta z_1 c_1^*} \left(\frac{D_m c^*}{\Delta z} \right)_{3/2} \quad (A26)$$

$$CDIFF_1 = \frac{2}{\Delta z_1 c^*_2} \left(\frac{D_m c^*}{\Delta z} \right)_{3/2} \quad (A27)$$

This form may be used in Equation (A11), which results in

$$BM_1 = \begin{bmatrix} 1 - \epsilon BDIFF_1 - \epsilon C1_1 + \frac{2w_{r1}}{\Delta z_1} & \frac{\epsilon}{\Delta z_1} \\ 2w_{v1} & 1 \end{bmatrix} \quad (A28)$$

$$CM_1 = \begin{bmatrix} -\epsilon CDIFF_1 & 0 \\ -2w_{v2} & 1 \end{bmatrix} \quad (A29)$$

$$DV_1 = \begin{bmatrix} c_1^j + \epsilon (BDIFF_1 c_1^j + CDIFF_1 c_2^j + C1_1 c_1^j + 2D1_1) \\ -\frac{2w_{r1}}{\Delta z_1} c_1^j - \frac{R_1^j}{\Delta z_1} + \frac{2}{\Delta z_1} (\hat{f}_B^j + \hat{f}_B^{j+1}) \\ 0 \end{bmatrix} \quad (A30)$$

The derivation for a flux boundary condition at the top grid point is similar. The diffusion term is developed as

$$\begin{aligned} \frac{\partial}{\partial z} \left[c^* D_m \frac{\partial}{\partial z} (c/c^*) \right]_n^j &= ADIFF_n c_{n-1}^j + BDIFF_n c_n^j \\ &+ \frac{2}{\Delta z_n} (w_{rc})_n^j - \frac{2}{\Delta z_n} \hat{f}_T^j \end{aligned} \quad (A31)$$

where

$$ADIFF_n = \frac{2}{\Delta z_n c_{n-1}^*} \left(\frac{D_m c^*}{\Delta z} \right)_{n-1/2} \quad (A32)$$

$$BDIFF_n = - \frac{2}{\Delta z_n c_n^*} \left(\frac{D_m c^*}{\Delta z} \right)_{n-1/2} \quad (A33)$$

The resulting forms for AM, BM and DV are

$$AM_n = \begin{bmatrix} -\epsilon ADIFF_n & 0 \\ 2w_{vn-1} & 1 \end{bmatrix} \quad (A34)$$

$$BM_n = \begin{bmatrix} 1 - \epsilon BDIFF_n - \epsilon Cl_n - \frac{2\epsilon w_{rn}}{\Delta z_n} & \frac{\epsilon}{\Delta z_n} \\ 2w_{vn} & 1 \end{bmatrix} \quad (A35)$$

$$DV_n = \begin{bmatrix} c_n^j + \epsilon \left(ADIFF_n c_{n-1}^j + BDIFF_n c_n^j + Cl_n c_n^j \right. \\ \left. + 2Dl_n + \frac{2w_{rn}}{\Delta z_n} c_n^j - \frac{R_n^j}{\Delta z_n} - \frac{2}{\Delta z_n} (\hat{f}_T^j + \hat{f}_T^{j+1}) \right) \\ 0 \end{bmatrix} \quad (A36)$$

For the case of the outflow condition at the bottom boundary, we use a modified form of Equation (A11) obtained by evaluating the diffusion term one grid-point "upstream" (at $i = 2$) and one step back in time. This yields

$$\begin{aligned}
c_1^{j+1} - c_1^j = & -\frac{\epsilon}{\Delta z_1} (R_1^{j+1} + R_1^j) + \epsilon \left[\text{ADIFF}_2 (c_1^j + c_1^{j-1}) \right. \\
& + \text{BDIFF}_2 (c_2^j + c_2^{j-1}) + \text{CDIFF}_2 (c_3^j + c_3^{j-1}) \left. \right] \\
& + \epsilon \text{Cl}_1 (c_1^{j+1} + c_1^j) + 2 \epsilon \text{Dl}_1^j
\end{aligned} \tag{A37}$$

With this we obtain the following forms for BM, CM and DV:

$$\text{BM}_1 = \begin{bmatrix} 1 - \epsilon \text{Cl}_1 & \frac{\epsilon}{2\Delta z_1} \\ 2w_{v1} & 1 \end{bmatrix} \tag{A38}$$

$$\text{CM}_1 = \begin{bmatrix} 0 & 0 \\ -2w_{v2} & 1 \end{bmatrix} \tag{A39}$$

$$\text{DV}_1 = \begin{bmatrix} c_1^j + \epsilon \left(\text{Cl}_1 c_1^j + 2\text{Dl}_1 - \frac{R_1^j}{\Delta z_1} + \text{OUTDIF} \right) \\ 0 \end{bmatrix} \tag{A40}$$

where

$$\begin{aligned}
\text{OUTDIF} = & \text{ADIFF}_2 (c_1^j + c_1^{j+1}) + \text{BDIFF}_2 (c_2^j + c_2^{j-1}) \\
& + \text{CDIFF}_2 (c_3^j + c_3^{j-1})
\end{aligned}$$

The integration procedure over a single time step can be outlined as follows. At time t_j , the c_i^j are known and w_r , w_A'' , D_m , c^* , etc. are evaluated by various Class I subroutines. The R_i^j are evaluated by solving equations (A4)-(A6). The derivatives $w_{A\xi}''$ and c_ξ^* are evaluated similarly, to give the Cl_i . Now the AM, BM, CM, and DV may be calculated.

Finally, Equation (A11) are solved to obtain c_i^{j+1} and R_i^{j+1} . This involves solving a set of paired simultaneous linear equations with a tridiagonal coefficient matrix, and a matrix form of the Thomas algorithm provides an efficient solution technique (Adams, 1975).

The treatment of the energy balance involves only minor modifications. The advection term is treated just as for the mass-balance equations, with the simplification that $w_r \equiv 0$ in this case. The diffusion term for the energy-balance equation can be treated as in the mass-balance equation, but the ADIFF, BDIFF, and CDIFF are somewhat different in form. The interested reader can find their definitions in the PLUVIUS subroutine TEMPF where they are computed. The C1 only uses the left term in Equation (A10). The D1 term is given by

$$D1 = w_A \Gamma - \frac{1}{c^* \chi} \frac{\partial}{\partial z} (c^* \chi D_H \Gamma)$$

The derivative here is evaluated by

$$\left[\frac{\partial}{\partial z} (c^* \chi D_H \Gamma) \right]_i = \frac{1}{\Delta z_i} \left[(c^* \chi \Gamma)_{i+1/2} D_{H_{i+1/2}} - (c^* \chi \Gamma)_{i-1/2} D_{H_{i-1/2}} \right]$$

and $(c^* \chi \Gamma)$ is evaluated at $i \pm 1/2$ by averaging its values at adjacent grid points.

One problem with this integration technique is the generation of high-wave number computational noise near steep gradient regions of the solution. Indeed, nearly all second-order and higher accuracy methods have this problem when the mass balance equation is dominated by the advection terms. In some cases, the noise may only be cosmetically undesirable, as when it generates small negative concentration values. In cases where the basic equation is nonlinear, the noise may grow unstably and completely contaminate the solution. This problem has arisen in our experience when

working with precipitation species: a nonlinearity arises because the settling velocity is dependent on the precipitation concentration.

To reduce this problem, a filtering step has been added to the code and is exercised after each advection-diffusion integration step. The nonlinear filtering method devised by Forrester (1977) is used, with values for the filter parameters as suggested by McRae et al. (1982). Our experience suggests that the filtering is necessary for species with significant vertical velocities (w_r or w_a'), but is not always required for species with small vertical velocities (if the eddy diffusivity is sufficiently large). In situations where it is desirable to maintain a very sharp gradient (e.g., across a cloud base) and noise is not a problem, it is preferable not to filter the solution for particular species. Thus, a filtering coefficient FILFAC has been included as an input parameter for each species. Specifying a zero value for this coefficient effectively turns off the filter for a species. For any particular application, the need for filtering is best determined by experimentation.

REFERENCES

Adams, Y. 1975. "A Hermitian Finite Difference Method for the Solution of Parabolic Equations." Comp. & Maths. with Appls. 1:393-406.

Adams, Y. 1977. "Highly Accurate Compact Implicit Methods and Boundary Conditions." J. Comp. Physics. 24:10-22.

Forrester, C. K. 1977. "Higher Order Monotonic Convective Difference Schemes." J. Comp. Physics. 23:1-22.

McRae, G.J., W. R. Goodin and J.H. Seinfeld. 1982. "Numerical Solution of the Atmospheric Diffusion Equation for Chemically Reacting Flows." J. Comp. Physics. 45:1-42.

APPENDIX B
TECHNIQUE FOR APPROXIMATION TO SOLUTIONS OF
ORDINARY DIFFERENTIAL EQUATIONS

The integration of the generation components of the mass and energy-balance equations [Equations (43) and (45)] involves the solution of NCOMP simultaneous, ordinary differential equations over a specified time interval at each of the vertical grid points. For many atmospheric chemistry problems, these equations are highly-coupled and strongly nonlinear, and thus require specially designed algorithms for their efficient solution. In PLUVIUS MOD 5.0, this task is performed by subroutine ODEINT.^(a)

Subroutine ODEINT is essentially a predictor-corrector code for approximating the solutions of simultaneous, ordinary differential equations of the form

$$\frac{dc_k}{dt} = g_k - \epsilon_k c_k \quad ; \quad (B1)$$

$$k = 1, 2, \dots, NCOMP \quad ;$$

where

c_k is the concentration of species k at time t ,

g_k is the generation rate of species k , and

ϵ_k is a pseudo first-order rate coefficient describing the decay of species k .

At any given time step the code segregates the members of equation set (B1) on the basis of the magnitudes of ϵ_k . If ϵ_k exceeds a set value [RATESF(K)], then Equation (B1) is considered to be stiff. Under these circumstances, an asymptotic or an exponentially-assisted integration technique is applied, at the discretion of the user. If the equation is not

(a) Table C-7 contains a listing of ODEINT.

considered stiff, then a conventional predictor-corrector algorithm is used. Values of RATESF(K) are set by the user in a DATA statement.

ODEINT will provide approximations to any form of Equation (B1), regardless of the set values of RATESF(K). Appropriate choice of these values is reflected primarily in the efficiency of the resulting calculation. If RATESF(K) is set too high, then conventional calculations will be applied preferentially, forcing an inordinately fine integration time step to be used. If RATESF(K) is set too low, then the stiff algorithms will be invoked preferentially with some loss of computational efficiency. Optimum efficiency will be attained with appropriate intermediate values of RATESF(K). These values are somewhat problem dependent; in a practical sense the user is best advised to initially set RATESF(K) conservatively low,^(a) assessing the impact of increases in this parameter on subsequent test runs.

The argument list for the subroutine is as follows:

ODEINT (I, TSTRTO, DTTOT, DTSUG, DTMAX)

I = vertical position index (ODEINT solves Equation (B1) at the single grid point specified by I, and thus is called repeatedly with I varying from 1 to N;

TSTRTO = value of the independent variable (time) at the start of the integration;

DTTOT = integration span of independent variable;

DTSUG = "suggested value" of initial time step. If DTSUG is set positive in the subroutine call, then this value will be the one utilized. If DTSUG is set negative, ODEINT will compute its own starting step size;

DTMAX = maximum allowable step size, which must be set prior to interrogating ODEINT.

Additional essential variables are supplied to ODEINT via COMMON statements. These variables include:

(a) A recommended starting point for atmospheric chemistry simulations is RATESF(K) = 0.1 sec⁻¹.

NCORR = number of passes to be taken through corrector in any given time step (recommend NCORR=1 for simple systems of equations, NCORR=3 for highly nonlinear or coupled equations);
 IEXP = function control for stiff calculations - = 1 for exponential, = 0 for asymptotic;
 EPS = desired error tolerance (see discussion of step-size control);
 CMIN(K) = vector of dependent-variable minimums; (i.e., user-chosen nonzero values below which $c_{i,k}$ can be considered insignificant);
 CERROR(K) = vector of dependent-variable values. Convergence error criterion is relaxed when dependent-variable values fall below CERROR;
 NCOMP = number of dependent variables in Equation (B1);
 NCNSTR = number of "constrained," or steady-state variables;
 NTOT = total number of chemical species (=NCOMP + NCNSTR);
 C(I,K) = vector of dependent variables in Equation (B1) plus constrained variables, ordered such that constrained variables follow the dependent variables;
 GGEN(K), = generation and decay rates of species k.
 GDEC(K)

The C(I,K) array represents the initial conditions, which must be supplied prior to any interrogation of ODEINT. Upon entry to ODEINT, concentrations at position I are transferred from the C(I,K) to a one-dimensional working array, CNN(K). At successful completion of the integration, the final concentration values are transferred back into the C(I,K) array.

The arrays GGEN(K) and GDEC(K) are defined in terms of Equation (B1) as follows:

$$GGEN(K) \equiv g_k$$

$$GDEC(K) \equiv \xi_k c_k$$

Updated values of these variables are computed via interrogation of the subroutine

GEN (I,IGCALC,TGEN,DTAU,JPASSO) ,

where I is the usual vertical-position index. IGCALC is a mode-control variable, defined as follows:

IGCALC $\leq$ 0: Only concentrations of constrained species (CNN(NCOMP+1), ... CNN(NTOT) are computed.

IGCALC > 0: Both constrained species and generation and decay rates are computed.

TGEN is the value of the independent variable (time).

DTAU is the current integration time-step within ODEINT.

JPASSO specifies whether GEN is being called from the predictor section (=1) or the corrector section (=2,3,..., on first, second, ..., corrector pass) of ODEINT.

Subroutine GEN must be supplied in appropriate form by the user prior to executing ODEINT. Units for GGEN and GDEC are moles/cm³ sec, consistent with the code's standard usage. Note that GEN works with concentrations in the CNN(K) array, rather than the C(I,K) array.

Primary output from the subroutine is also conveyed via COMMON statements. In addition to the C(I,K) solution array, this includes the array DTSAVE(I), which is the most recent independent-variable increment. It is often convenient to use DTSAVE(I) as an initial increment on subsequent calls to ODEINT.

ODEINT is based on some of the concepts utilized in the CHEMEQ code prepared by Young (1980). The conventional (non-stiff) predictor-corrector algorithm in ODEINT is similar to that in CHEMEQ. The asymptotic corrector equations are substantially different, however, and represent a marked improvement in the overall technique.

Conventional predictor-corrector equations used by ODEINT correspond to the so-called "improved Euler's method" [Carnahan, Luther and Wilkes (1969)]. These are:

Predictor

$$c_{t+\Delta t}^1 = (g_t - \xi c_t) \Delta t + c_t ; \quad (B2)$$

Corrector

$$c_{t+\Delta t}^{m+1} = \left[\bar{g} - \frac{\bar{\xi}}{2} (c_t + c_{t+\Delta t}^m) \right] \Delta t + c_t . \quad (B3)$$

Equations (B2) and (B3) may be obtained directly from Equation (B1), dropping the k subscript for convenience. In these equations the superscript denotes the number of computational passes, and $\bar{g}$ and $\bar{\xi}$ pertain to simple averages over the interval Δt .

Exponential counterparts to Equations (B2) and (B3) can be derived by formally integrating Equation (B1) over the interval Δt , presuming that g_t and ξ_t are constant. The result is

$$c_{t+\Delta t}^1 = \frac{(g_t - \xi_t c_t) [\exp(\xi_t \Delta t) - 1]}{\xi_t \exp(\xi_t \Delta t)} + c_t \quad (B4)$$

which can be modified to a corrector form

$$c_{t+\Delta t}^{m+1} = \frac{(\bar{g} - \xi c_t) [\exp(\bar{\xi} \Delta t) - 1]}{\bar{\xi} \exp(\bar{\xi} \Delta t)} + c_t . \quad (B5)$$

One should note at this point, however, that in contrast to Equation (B3), concentration-averaging has not been performed to obtain Equation (B5). In this sense Equation (B5) should be considered more as an "improved predictor" than an actual corrector counterpart to Equation (B3).

Asymptotic approximations to Equations (B4) and (B5) can be derived by approximating $\exp(\xi \Delta t)$ in a Taylor's series:

$$\exp(\xi \Delta t) = 1 + \xi \Delta t + \frac{\xi^2 (\Delta t)^2}{2!} + \dots \quad (B6)$$

Truncation of Equation (B6) after the second and third terms leads respectively to the following asymptotic counterparts to Equations (B4) and (B5):

Predictor:

$$c_{t+\Delta t}^1 = \frac{(g_t - c_t \xi_t) \Delta t}{1 + \xi_t \Delta t} + c_t ; \quad (B7)$$

Corrector:

$$c_{t+\Delta t}^{m+1} = \frac{(\bar{g} - c_t \bar{\xi}) \Delta t \left(1 + \frac{\xi \Delta t}{2}\right)}{1 + \xi \Delta t \left(1 + \frac{\xi \Delta t}{2}\right)} + c_t ; \quad (B8)$$

The additional Taylor's-series term has been included in Equation (B8) as a practical method of establishing conservative step-size control in the associated numerical algorithm.

Choice between exponentially-assisted or asymptotic calculations (IEXP=1 or 0, respectively) is at the user's discretion. The asymptotic forms Equations (B7) and (B8) pose the computational advantage of not requiring transcendental functions; the exponential counterparts, on the other hand, may be considered as somewhat more accurate (for any given step size), especially for reactions exhibiting a true first-order decay.

Choice of the appropriate number of corrector passes (NCORR) is also up to the user's discretion, and depends primarily upon system complexity. Simple noninteractive systems should be treated with a single corrector pass, while for highly interactive systems triple corrector passes may be advantageous. Multiple corrector passes provide the opportunity for enhanced dialogue between equations in the family at the expense of increased computation time Equation (B1). In general, an odd number of corrector passes will provide superior computational performance; using NCORR>3 is not recommended for any practical application.

Step-size control in ODEINT is determined primarily by the disagreement in values of the dependent variable(s) arising from the predictor and corrector

operations of the previous time step. Since the error associated with Equations (B2) and (B3) is of the order of $(\Delta t)^2$:

$$\text{ERROR} \approx_{\alpha} (\Delta t)^2 ; \alpha = \text{some constant} .$$

If ϵ_{old} is the error associated with the previous time step, and EPS is the desired error tolerance, then

$$\epsilon_{\text{old}} \approx_{\alpha} (\Delta t_{\text{old}})^2$$

and $\text{EPS} \approx_{\alpha} (\Delta t_{\text{new}})^2 ;$

thus
$$\Delta t_{\text{new}} = \Delta t_{\text{old}} \sqrt{\frac{\text{EPS}}{\epsilon_{\text{old}}}} \quad (\text{B9})$$

Equation (B9), modified by a 0.9 conservatism factor, is used as a primary means of step-size control in ODEINT.

Under conditions where a given predictor-corrector cycle fails to achieve convergence, a penalty factor, PFACT = 0.5 is imposed on the system. This reduces the subsequent grid step to one half of its naturally-computed value. In succeeding, successful cycles PFACT gradually approaches 1.0, thus effecting a gradual relaxation of the penalty.

Under conditions where conventional predictor-corrector solution becomes negative for any dependent variable, the complete set of calculations for that time step is abandoned, and calculations are restarted for one-half the unsuccessful grid size. (The exponential and asymptotic approximations are always non-negative).

Error-relaxation is applied within the algorithm under circumstances when relative errors are insignificant. Four different situations where such relaxation occurs are:

- whenever concentrations approach negligible values (less than CERROR),

- whenever the starting concentration (c_t) is negligibly small (near CMIN),
- whenever the projected concentration increase is so great as to make the current value and its relative error small by comparison, and
- whenever the projected concentration decrease is extremely rapid and a negligible concentration (near CMIN) will be reached shortly.

Error relaxation in this manner increases computational speed significantly. The user should review these adjustments in light of his individual needs however, and should modify the subroutine's relaxation block to fit his own particular requirements.

REFERENCES

Carnahan, B., H. A. Luther and J. O. Wilkes. 1969. Applied Numerical Methods. John Wiley, New York.

Young, T. R. 1980. CHEMEQ - A Subroutine for Solving Stiff Ordinary Differential Equations. NRL Memorandum Report 4091, Naval Research Laboratory, Washington, D.C.

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APPENDIX C

PLUVIUS MAIN PROGRAM AND CLASS II SUBROUTINE LISTINGS

This appendix contains listings of the PLUVIUS main program and the 17 Class II subroutines. Note that most of these program units reference an INCLUDE file like that in Table 3-2 or Table 5-4. Table C-19 contains a description of variables and parameters that appear in the code.

TABLE C-1. Listing of PLUVIUS Main Program Unit

```
C
C PLUVIUS MOD 5
C
C VERSION 1 - RELEASED AUG 1984
C
C FOR DOCUMENTATION SEE:
C   J.M. HALES AND R.C. EASTER. PLUVIUS MOD 5 USER'S MANUAL.
C   PACIFIC NORTHWEST LABORATORIES REPORT TO U.S. EPA,
C   AUGUST, 1984 (**DRAFT**)
C
C FOR INFORMATION, CONTACT:
C   J.M. HALES OR R.C. EASTER
C   GEOSCIENCES RESEARCH AND ENGINEERING DEPT.
C   BATTELLE PACIFIC NORTHWEST LABORATORIES
C   P.O. BOX 999
C   RICHLAND, WA. 99352
C
C-----
C
C LANGUAGE: FORTRAN-77.
C
C THIS CODE WAS DEVELOPED ON A VAX 11-780 USING THE VMS OPERATING
C SYSTEM. THE PROGRAM USES NO OPERATING SYSTEM FACILITIES.
C THE ONLY CHANGES NEEDED TO RUN IT ON ANOTHER SYSTEM ARE THE
C FOLLOWING NON-STANDARD LANGUAGE USAGES (FROM DEC VAX FORTRAN-77):
C   1. THE "INCLUDE" STATEMENT, FOUND AT THE START OF EACH PROGRAM UNIT
C
C-----
C
C   PROGRAM PLUVIUS
C
C   INCLUDE 'PLUVCMN'
C
C   COMMON/FILTERCMN/NFILTR,FILFAC(NCMAX),MAXITA,MAXITB,NFSRCH,NFSET
C
C-----
C
C   INPUT SECTION
C
C-----
C
C   READ (LUNIN,9000) MTITLE
C   READ (LUNIN,9010) NCOMP,NCNSTR
C   NTOT=NCOMP+NCNSTR
C   IF ((NCOMP.GT.NCMAX) .OR. (NTOT.GT.NCTMAX)) STOP 9990
C   IF ((NCOMP.LT.1) .OR. (NCNSTR.LT.0)) STOP 9991
```


TABLE C-1 Continued

```

DO K=1,NTOT
  READ (LUNIN,9000) (NAME(LL,K),LL=1,5)
END DO
READ (LUNIN,9020) N,LTD,DZ,GLEVL
IF ((N.GT.NZMAX) .OR. (LTD.GT.4)) STOP 9992
IF ((N.LT.1) .OR. (LTD.LT.1)) STOP 9993

READ (LUNIN,9030) TSTART,TSTOP,DT
READ (LUNIN,9040) NPRINT,DTPRIN,ITCOLL,DTCOLL
READ (LUNIN,9010) IGEN,IDIFF,ITEMP,IPRESS,ISSETL,IBOUND,IVERT,
2   IFOG,ISHEAR
DO K=1,NCOMP
  READ (LUNIN,9050) ITOP(K),IBOT(K),LDIF(K),FILFAC(K)
END DO
READ (LUNIN,9030) PRESS0, TEMP0

9000  FORMAT (40A2)
9010  FORMAT (10I5)
9020  FORMAT(2I5,2E10.3)
9030  FORMAT(3E10.3)
9040  FORMAT(I5,E10.3,I5,E10.3)
9050  FORMAT(3I5,E10.3)

```

```

C-----
C
C   INITIALIZATION OPERATIONS
C
C-----

```

```

NM1=N-1
CALL GRDSET
DO I = 2, NM1
  DZDIZ(I) = 0.5*(Z(I+1) - Z(I-1))
END DO
DZDIZ(1) = Z(2) - Z(1)
DZDIZ(N) = Z(N) - Z(NM1)

DTOLD=DT
TCLOCK=TSTART
TNEXT=TCLOCK
IF (NPRINT .GT. 0) THEN
  IPRINT=0
ELSE
  IPRINT = NPRINT - 1
END IF
IF (DTPRIN .GT. 0.) THEN
  TPRINT = TCLOCK + DTPRIN

```

TABLE C-1 Continued

```

ELSE
  TPRINT = TSTOP + 1.E5
END IF
ISLDER = IDIFF + IVERT + ITEMP + IPRESS
C
C
  INIT = 1
  INITBB = 1
  CALL USHEAR (INIT)
  CALL SETUP (INIT)
  DO I = 1, N
    DO K = 1, NTOT
      CNN(K) = AMAX1( C(I,K), CMIN(K) )
    END DO
    CALL GEN( I, 0, TCLOCK, 2.*DT, 1 )
    DO K = 1, NTOT
      C(I,K) = CNN(K)
    END DO
  END DO
  CALL DIFF (INIT)
  CALL VERT (INIT)
  CALL SETTL (INIT)
  CALL FILTER (INIT)
  IF (N .GE. 3) CALL BOUND (INIT)

  CALL PRINT( INIT, TSTART, TSTOP, NPRINT, DTPRIN, DTCOLL )
  IF (ITCOLL .NE. 0) CALL COLLECT (INIT, ITCOLL, DTCOLL)

  INIT=0

C-----
C
C
C  MAIN COMPUTATIONAL LOOP - INTEGRATES THE MASS BALANCE EQUATIONS OVER
C  A TIME STEP OF 2*DT
C
C-----
1000  CONTINUE

C
C  SAVE CONCENTRATIONS AND BOUNDARY CONDS.
C
  DO K = 1, NTOT
    DO I = 1, N
      COLD(I,K) = C(I,K)
    
```

TABLE C-1 Continued

```

      END DO
    END DO
    DO K = 1, NCOMP
      FBOLD(K) = FB(K)
      FTOLD(K) = FT(K)
    END DO

```

```

C
C DO ADVECTION-DIFFUSION INTEGRATION FOR TIME STEP DT
C

```

```

      IF (ISHEAR .NE. 0) CALL USHEAR( INIT )
      IF (IDIFF .NE. 0) CALL DIFF ( INIT )
      IF (IVERT .NE. 0) CALL VERT( INIT )
      IF (ISETTL .NE. 0) CALL SETTLE( INIT )
      DTOLD = DT
      CALL TIMESP
      TNEXT = TCLOCK + DT

      CALL ADVINT( INIT, INITBB, ISLDER )
      CALL ADJUST
      TCMID = TNEXT

```

```

C
C DO CHEMICAL REACTION / MASS TRANSFER INTEGRATION FOR TIME STEP 2*DT
C

```

```

      IF (IGEN .NE. 0) CALL CHMINT( INIT, INITBB )

```

```

C
C SAVE CONCENTRATIONS AND BOUNDARY CONDS. AGAIN
C

```

```

      TCLOCK = TCMID
      TNEXT = TCMID
      INITBB = 0
      DO K = 1, NTOT
        DO I = 1, N
          COLD(I,K) = C(I,K)
        END DO
      END DO
      DO K = 1, NCOMP
        FBOLD(K) = FB(K)
        FTOLD(K) = FT(K)
      END DO

```

```

C
C DO ADVECTION-DIFFUSION INTEGRATION FOR TIME STEP DT AGAIN
C

```

TABLE C-1 Continued

```

IF (ISHEAR .NE. 0) CALL USHEAR( INIT )
IF (IDIFF .NE. 0) CALL DIFF ( INIT )
IF (IVERT .NE. 0) CALL VERT( INIT )
IF (ISETTL .NE. 0) CALL SETTL( INIT )
TNEXT = TCLOCK + DT

CALL ADVINT( INIT, INITBB, ISLDER )
CALL ADJUST
TCLOCK = TNEXT

C
C
C OUTPUT RESULTS
C
C
IF (ITCOLL .NE. 0) CALL COLLECT (INIT, ITCOLL, DTCOLL)

IF (NPRINT .GT. 0) IPRINT = IPRINT+1
IF ( (TCLOCK.GE.TSTOP) .OR. (IPRINT.EQ.NPRINT)
+   .OR. (TCLOCK.GE.TPRINT) ) THEN
  DO I = 1, N
    DO K = 1, NTOT
      CNN(K) = AMAX1( C(I,K), CMIN(K) )
    END DO
    CALL GEN( I, 0, TCLOCK, 2.*DT, 1 )
    DO K = 1, NTOT
      C(I,K) = CNN(K)
    END DO
  END DO
  CALL PRINT( INIT, TSTART, TSTOP, NPRINT, DTPRIN, DTCOLL )
  IF (NPRINT .GT. 0) IPRINT = 0
  IF (DTPRIN .GT. 0.) TPRINT = TPRINT + DTPRIN
END IF

C
C CHECK FOR COMPLETION / REPEAT MAIN LOOP
C
IF (TCLOCK.LT.TSTOP) GOTO 1000

C
C ALL DONE
C
INIT = -1
IF (ITCOLL .NE. 0) CALL COLLECT (INIT, ITCOLL, DTCOLL)
STOP
END

```

TABLE C-2. Listing of Subroutine ADVINT

```

SUBROUTINE ADVINT( INIT, INITBB, ISLDER )
C
C ROUTINE PERFORMS SINGLE TIME STEP INTEGRATION OF ADVECTION-DIFFUSION
C PORTION OF MASS BALANCE EQUATION
C

INCLUDE 'PLUVCMN'
DIMENSION DC2OUT(NCMAX)

C
C DEGENERATE GRID COMPUTATIONS
C
IF (N .LT. 3) THEN
    GLEVL = GLEVL + DT*URATIO(1)*WAGRID(1)
    CALL ZERODM( INITBB )
    RETURN
END IF

C SET BOUNDARY CONDITIONS
IF (IBOUND .NE. 0) CALL BOUND( INIT )
IF (ISLDER+INITBB .NE. 0) CALL DERIV( INITBB )

C
C LOOP FOR EACH COMPUTED SPECIES
C
DO 4000 K = 1, NCOMP
    L = LDIF(K)

C
C CALCULATE FIRST DERIVATIVE OF C*(WR + WAP)
C
DO I = 1, N
    WVAR(I) = WR(I,K) + WAP(I)
    DWVCDI(I) = WVAR(I)*COLD(I,K)
END DO
CALL FIRSTD( DWVCDI, DWVCDI )

C
C GET DIFF. EQUATION AND BOUNDARY RELATION COEFFICIENTS
C
IF (K.EQ.KTEMP) THEN
    IF (ITEMP .EQ. 0) GOTO 4000
    CALL TEMPF( FXBTC1, FXBTD1, FXTPC1, FXTPD1 )

```

TABLE C-2 Continued

```

ELSE
  CALL SETVEC( K, FXBTC1, FXBD1, FXTPC1, FXTPD1 )
END IF

```

C
C
C

SET UP INTERIOR TRI-DIAGONAL COEFFICIENTS

```

DO I = 2, NM1
  DTHFUR = .5*DT*URATIO(I)
  AMAT(2,1,I) = 3.*WVAR(I-1)
  AMAT(2,2,I) = 1.
  AMAT(1,1,I) = - DTHFUR*ADIFFU(I,L)
  AMAT(1,2,I) = 0.

  BMAT(2,1,I) = 0.
  BMAT(2,2,I) = 4.
  BMAT(1,1,I) = 1.0 - DTHFUR*C1(I) - DTHFUR*BDIFFU(I,L)
  BMAT(1,2,I) = DTHFUR/DZDIZ(I)

  CMAT(2,1,I) = -3.*WVAR(I+1)
  CMAT(2,2,I) = 1.
  CMAT(1,1,I) = - DTHFUR*CDIFFU(I,L)
  CMAT(1,2,I) = 0.0

  DVEC(2,I) = 0.
  DVEC(1,I) = COLD(I,K) + DTHFUR*( -DWVCDI(I)/DZDIZ(I) +
+      2.*D1ADV(I) + (C1(I) + BDIFFU(I,L))*COLD(I,K) +
+      ADIFFU(I,L)*COLD(I-1,K) + CDIFFU(I,L)*COLD(I+1,K) )
END DO

```

C
C
C

SET UP TRI-DIAGONAL COEFFICIENTS TOP BOUNDARY

C
C

SECOND COMPONENT OF THE COEFFICIENTS

```

AMAT(2,1,N) = 2.*WVAR(NM1)
AMAT(2,2,N) = 1.
BMAT(2,1,N) = -2.*WVAR(N)
BMAT(2,2,N) = 1.
DVEC(2,N) = 0.

```

C

TABLE C-2 Continued

```

C  FIRST COMPONENT - INFLOW OR "CONCENTRATION" BOUNDARY CONDITION
    IF (ITOP(K) .LE. 0) THEN
        AMAT(1,1,N) = 0.
        AMAT(1,2,N) = 0.
        BMAT(1,1,N) = 1.
        BMAT(1,2,N) = 0.
        DVEC(1,N) = CT(K)

C
C  FIRST COMPONENT - FLUX BOUNDARY CONDITION
    ELSE
        DTHFUR = .5*DT*URATIO(N)
        AMAT(1,1,N) = - DTHFUR*ADIFFU(N,L)
        AMAT(1,2,N) = 0.
        BMAT(1,1,N) = 1.0 - DTHFUR*( C1(N) + BDIFFU(N,L) + FXTPC1 )
        BMAT(1,2,N) = DTHFUR/DZDIZ(N)
        DVEC(1,N) = COLD(N,K) + DTHFUR*( -(DWVCDI(N)/DZDIZ(N))
+           + COLD(N,K)*( C1(N) + BDIFFU(N,L) + FXTPC1 )
+           + COLD(NM1,K)*ADIFFU(N,L) + 2.0*( D1ADV(N) + FXTPD1 ) )

    END IF

C
C  SET UP TRI-DIAGONAL COEFFICIENTS AT BOTTOM BOUNDARY
C

C
C  SECOND COMPONENT OF THE COEFFICIENTS
    BMAT(2,1,1) = 2.*WVAR(1)
    BMAT(2,2,1) = 1.
    CMAT(2,1,1) = -2.*WVAR(2)
    CMAT(2,2,1) = 1.
    DVEC(2,1) = 0.

C
C  FIRST COMPONENT - INFLOW OR "CONCENTRATION" BOUNDARY CONDITION
    IF (IBOT(K) .EQ. 0) THEN
        BMAT(1,1,1) = 1.
        BMAT(1,2,1) = 0.
        CMAT(1,1,1) = 0.
        CMAT(1,2,1) = 0.
        DVEC(1,1) = CB(K)

C
C  FIRST COMPONENT - OUTFLOW BOUNDARY CONDITION
    ELSE IF (IBOT(K) .LT. 0) THEN

```

TABLE C-2 Continued

```

DTHFUR = .5*DT*URATIO(1)
DC2OUX = ADIFFU(2,L)*COLD(1,K) + BDIFFU(2,L)*COLD(2,K) +
+       CDIFFU(2,L)*COLD(3,K)
IF (INITBB .NE. 0) DC2OUT(K) = DC2OUX
CMAT(1,2,1) = 0.

C
C   CHECK THAT W IS ACTUALLY OUTFLOW
IF (WVAR(1) .LT. 0.) THEN
    BMAT(1,1,1) = 1. - DTHFUR*C1(1)
    BMAT(1,2,1) = DTHFUR/DZDIZ(1)
    CMAT(1,1,1) = 0.
    DVEC(1,1) = COLD(1,K) + DTHFUR*( -(DWVCDI(1)/DZDIZ(1))
+       + C1(1)*COLD(1,K) + 2.*D1ADV(1)
+       + DC2OUX + DC2OUT(K) )
ELSE
C
C   HAVE INFLOW, USE DC/DZ = 0 AS THE B.C. ( C(2) = C(1) )
    BMAT(1,1,1) = 1.
    BMAT(1,2,1) = 0.
    CMAT(1,1,1) = -1.
    DVEC(1,1) = 0.
    END IF

    DC2OUT(K) = DC2OUX

C
C   FIRST COMPONENT, FLUX BOUNDARY CONDITION
ELSE
    DTHFUR = .5*DT*URATIO(1)
    BMAT(1,1,1) = 1.0 - DTHFUR*( C1(1) + BDIFFU(1,L) + FXBTC1 )
    BMAT(1,2,1) = DTHFUR/DZDIZ(1)
    CMAT(1,1,1) = - DTHFUR*CDIFFU(1,L)
    CMAT(1,2,1) = 0.
    DVEC(1,1) = COLD(1,K) + DTHFUR*( - (DWVCDI(1)/DZDIZ(1))
+       + COLD(1,K)*( C1(1) + BDIFFU(1,L) + FXBTC1 )
+       + COLD(2,K)*CDIFFU(1,L) + 2.*( D1ADV(1) + FXBTD1 ) )

    END IF

C
C   SOLVE TRI-DIAGONAL SYSTEM FOR NEW C'S AND DCDZ'S
CALL TRIDG2( 1, N, AMAT, BMAT, CMAT, DVEC, UVEC )
DO I = 1, N
    C(I,K) = UVEC(1,I)
END DO

```


TABLE C-2 Continued

4000 CONTINUE

C
C APPLY FILTER TO SOLUTION VARIABLES
C
CALL FILTER(INIT)

C
C CALC NEW SURFACE LEVEL AND PRESSURE
C

GLEVL = GLEVL + DT*URATIO(1)*WAGRID(1)
IF (IPRESS .NE. 0) CALL PRESSF(INIT)

RETURN
END

TABLE C-3. Listing of Subroutine CHMINT

```

C      SUBROUTINE CHMINT( INIT, INITBB )
C
C      ROUTINE PERFORMS SINGLE TIME STEP INTEGRATION OF CHEMICAL REACTION
C      AND INTER-PHASE TRANSFER PORTION OF MASS BALANCE EQUATION
C
      INCLUDE 'PLUVCMN'
      TWODT = 2.0*DT
      TCLSAV = TCLOCK
      DO I = 1, N
        IF (INITBB .EQ. 0) THEN
          DTSUG = DTSAVE(I)
        ELSE
          DTSUG = -1.0
        END IF
        CALL ODEINT( I, TCLOCK, TWODT, DTSUG, TWODT )
        TCLOCK = TCLSAV
      END DO
      RETURN
      END

```

TABLE C-4. Listing of Subroutine DERIV

```

C      SUBROUTINE DERIV (INIT)
C
C      DERIV CALCULATES COEFFICIENTS USED DURING THE ADVECTION-DIFFUSION
C      INTEGRATION STEP WHICH ARE "SPECIES INDEPENDENT"
C
C      INCLUDE 'PLUVCMN'
C
C
C      CALCULATE ADIFFU, BDIFFU, CDIFFU
C
C      THE ADIFFU, BDIFFU, CDIFFU ARE DEFINED BY
C
C      D      D      C
C      -- (  DIFFUS  *  CS  *  - (  -- )  )  AT GRID I
C      DZ      DZ      CS
C
C      =  ADIFFU(I)*C(I-1) + BDIFFU(I)*C(I) + CDIFFU(I)*Q(I+1)
C
C      CONVENTION FOR DIFFUSIVITIES:
C      D(I, ) IS DIFFUSIVITY AT GRID I+1/2
C
C      DHATIP = DIFFUSIVITY(I+1/2) / DZ(I+1/2)
C      DHATIM = DIFFUSIVITY(I-1/2) / DZ(I-1/2)
C
C      DZ = "LAYER WIDTH"
C      DZ(I+1/2) = Z(I+1) - Z(I)
C      DZ(I) = DZDIZ(I) = .5*(Z(I+1) - Z(I-1))
C
C      EXCEPT:  DZDIZ(1) = Z(2) - Z(1)
C      DZDIZ(N) = Z(N) - Z(NM1)
C
C      DO L = 1, LTD
C
C          DHATIP = D(1,L)/DZDIZ(1)
C          CDIFFU(1,L) = DHATIP*(1. + CS(1)/CS(2))/(DZDIZ(1))
C          BDIFFU(1,L) = -DHATIP*(1. + CS(2)/CS(1))/(DZDIZ(1))
C          ADIFFU(1,L) = 0.
C
C          DO I = 2, NM1
C              IP1 = I+1
C              IM1 = I-1
C              TWODH = 2.*DZDIZ(I)
C              DHATIM = DHATIP
C              DHATIP = D(I,L)/(Z(IP1) - Z(I))

```

TABLE C-4 Continued

```

ADIFFU(I,L) = DHATIM*(1. + CS(I)/CS(IM1))/TWODH
CDIFFU(I,L) = DHATIP*(1. + CS(I)/CS(IP1))/TWODH

+ BDIFFU(I,L) = -( DHATIM*(1. + CS(IM1)/CS(I)) +
DHATIP*(1. + CS(IP1)/CS(I)) )/TWODH

```

END DO

```

CDIFFU(N,L) = 0.
BDIFFU(N,L) = -DHATIP*(1. + CS(NM1)/CS(N))/(DZDIZ(N))
ADIFFU(N,L) = DHATIP*(1. + CS(N)/CS(NM1))/(DZDIZ(N))

```

END DO

C
C
C
C
C
C
C
C

COMPUTE:

```

C1DWAP = D( WAP )/DZ = (1./DZDIZ) * D( WAP )/DIZ
C1DLCS = (WA / CS) * D( CS )/DZ
        = ((WAGRID+WAP) / CS / DZDIZ) * D( CS )/DIZ

```

```

CALL FIRSTD( WAP, C1DWAP )
CALL FIRSTD( CS, C1DLCS )

```

```

DO I = 1, N
  C1DWAP(I) = C1DWAP(I)/DZDIZ(I)
  C1DLCS(I) = (WAGRID(I)+WAP(I))*C1DLCS(I)/(CS(I)*DZDIZ(I))
END DO

```

```

RETURN
END

```

TABLE C-5. Listing of Subroutine FILTER

```

C      SUBROUTINE FILTER( INIT )
C
C      FILE FILTER53
C
C      APPLIES NON-LINEAR FILTER OF C.K.FORESTER (J.COMP.PHYS, 1977, PP 1-22)
C      WITH FOLLOWING CHANGES:
C          1. MODIFIED TO BE MASS CONSERVATIVE FOR NON-UNIFORM GRIDS
C          2. FOR FLUX BOUNDARY CONDITION AT TOP BOUNDARY, FILTERING IS DONE
C              WHENEVER CONCENTRATION AT TOP GRID POINT IS NEGATIVE
C
C      VARIABLES:
C          PHIFIL - PHI IN FORESTER'S PAPER
C          SFIL - S IN FORESTER'S PAPER
C
C      CONSTANTS:
C          NFILTR - FILTERING OCCURS EVERY NFILTR TIME STEPS
C          MAXITA, MAXITB - MAXIMUM NO. OF FILTER ITERATIONS FOR COURANT NUMBER
C                          GREATER-THAN, LESS-THAN 0.5
C          NLARGE - MUST HAVE THIS MANY GRID POINTS WITH LOCAL COURANT NO. GREATER
C                  THAN 0.5 TO USE MAXITA ITERATIONS
C          NFSRCH, NFSET - N AND M IN FORESTER'S PAPER
C          FILFAC - 0.5*MU IN FORESTER'S PAPER
C                  SPECIFIED BY USER FOR EACH SPECIES. SUGGESTED VALUES ARE
C                  0.1 FOR FILTERED SPECIES, 0.0 FOR NON-FILTERED SPECIES
C
C      INCLUDE 'PLUVCMN'
C
C      COMMON / FILTERCMN / NFILTR, FILFAC(NCMAX), MAXITA, MAXITB,
+      NFSRCH,NFSET
C
C      DIMENSION PHIFIL(NZMAX), SFIL(NZMAX), DELC(NZMAX)
C      EQUIVALENCE (SFIL(1), DELC(1))
C      LOGICAL NOISE,INOISE
C
C      DATA NLARGE / 3 /
C      DATA NFILTR / 1 /
C      DATA MAXITA, MAXITB / 3, 2 /
C      DATA NFSRCH, NFSET / 4, 2 /
C
C      INITIAL PASS - SET UP CONSTANTS
C
C      IF (INIT .EQ. 0) GO TO 20000
C      IFILTR = 0
C      RETURN
C

```

TABLE C-5 Continued

```

C   SUBSEQUENT PASSES - CHECK IF NFILTR TIME STEPS HAVE PASSES
C
2000  IFILTR = MOD(IFILTR+1, NFILTR)
      IF (IFILTR .NE. 0) RETURN
C
C   APPLY FILTER
C
C   LOOP OVER EACH SPECIES
C
      DO 6000 K = 1, NCOMP
        IF (FILFAC(K) .LE. 0.) GO TO 6000
C
C   CALC COURANT NO. TO DETERMINE NO. OF ITERATIONS
C
      ILARGE = 0
      DO I = 1, N
        IA = MIN0(I, NM1)
        COUNO = URATIO(I)*(WR(I,K) + WAP(I))*DT/(Z(IA+1)-Z(IA))
        IF (COUNO .GT. 0.5) ILARGE = ILARGE+1
      END DO
      IF (ILARGE .GE. NLARGE) THEN
        MAXITR = MAXITA
      ELSE
        MAXITR = MAXITB
      END IF
C
C   NOW ITERATE THAT MANY ITERATIONS OR UNTIL NO NOISE
C
      NITR = 0
      NOISE = .TRUE.
      DO WHILE ((NITR.LT.MAXITR) .AND. NOISE)
C
C   SET PHI'S TO ZERO AND CALC. THE S'S
C
        NOISE = .FALSE.
        DO I = 1, N
          PHIFIL(I) = 0.
        END DO
        DO I = 2, N
          IF (C(I,K) .GE. C(I-1,K)) THEN
            SFIL(I) = 1.0
          
```

TABLE C-5 Continued

```

ELSE
  SFIL(I) = -1.0
END IF
END DO

C
C NOW CHECK FOR NOISY DATA POINTS AND SET PHI'S AS NEEDED
DO I = 2, NM1
  IF (SFIL(I) .NE. SFIL(I+1)) THEN
    INOISE = .FALSE.
    J = 1
    DO WHILE ((.NOT.INOISE) .AND. (J.LE.NFSRCH))
      IA = I-J
      IF (IA .GE. 2) THEN
        IF (SFIL(IA) .NE. SFIL(I)) THEN
          INOISE = .TRUE.
        END IF
      END IF
      IA = I+1+J
      IF (IA .LE. N) THEN
        IF (SFIL(IA) .NE. SFIL(I+1)) THEN
          INOISE = .TRUE.
        END IF
      END IF
      J = J+1
    END DO

    IF ( INOISE ) THEN
      NOISE = .TRUE.
      JA = MAX0(1, I-NFSET)
      JB = MIN0(N, I+NFSET)
      DO J = JA, JB
        PHIFIL(J) = 1.
      END DO
    END IF
  END IF
END DO

IF (ITOP(K) .GT. 0) THEN
  IF (C(N,K) .LT. 0.) THEN
    PHIFIL(NM1) = 1.
    PHIFIL(N) = 1.
    NOISE = .TRUE.
  END IF
END IF

C
C DO SMOOTHING IF ANY NOISY POINTS FOUND
C

```

TABLE C-5 Continued

```

      IF ( NOISE ) THEN
        DO I = 1, NM1
          DELC(I) = FILFAC(K) * (C(I+1,K) - C(I,K)) *
+          (PHIFIL(I+1) ÷ PHIFIL(I)) * (Z(I+1) - Z(I))
        END DO
        C(1,K) = C(1,K) + DELC(1)/(0.5*DZDIZ(1))
        C(N,K) = C(N,K) - DELC(NM1)/(0.5*DZDIZ(N))
        DO I = 2, NM1
          C(I,K) = C(I,K) + (DELC(I) - DELC(I-1))/DZDIZ(I)
        END DO
      END IF

      NITR = NITR + 1
    END DO

6000  END DO

    RETURN
  END

```


TABLE C-6. Listing of Subroutine FIRSTD

```

C      SUBROUTINE FIRSTD( Q, DQDIZ )
C
C      CALCULATES THE VERTICAL DERIVATIVE OF A "FUNCTION"
C      OR SPECIES HELD IN THE ARRAY Q
C      THE DERIVATIVES ARE RETURNED IN THE ARRAY DQDIZ
C
C      DQDIZ IS THE DERIVATIVE WITH RESPECT TO THE GRID VARIABLE "IZ"
C      IT IS RELATED TO THE TRUE VERTICAL DERIVATIVE, DQDZ, BY
C          DQDZ = DQDIZ / DZDIZ
C
C      THE DQDIZ ARE SPECIFIED BY A SET OF LINEAR EQUATIONS.  THE
C      COEFFICIENT MATRIX IS TRIDIAGONAL, AND IS SOLVED USING
C      THOMAS'S ALGORITHM
C
C      USES WORKING ARRAYS ADUM, BDUM, CDUM, DDUM, WHICH OVERWRITE THE
C      AMAT, BMAT, CMAT, DVEC ARRAYS IN COMMON
C
C      INCLUDE 'PLUVCMN'
C
C      DIMENSION ADUM(NZMAX), BDUM(NZMAX), CDUM(NZMAX), DDUM(NZMAX)
C      EQUIVALENCE (ADUM(1), AMAT(1,1,1))
C      EQUIVALENCE (BDUM(1), BMAT(1,1,1))
C      EQUIVALENCE (CDUM(1), CMAT(1,1,1))
C      EQUIVALENCE (DDUM(1), DVEC(1,1))
C      DIMENSION Q(N), DQDIZ(N)
C
C      IF (N .LT. 3) RETURN
C
C      DO I = 2, NM1
C          ADUM(I) = 1.
C          BDUM(I) = 4.
C          CDUM(I) = 1.
C          DDUM(I) = 3.*( Q(I+1) - Q(I-1) )
C      END DO
C
C      ADUM(1) = 0.
C      BDUM(1) = 1.
C      CDUM(1) = 1.
C      DDUM(1) = 2.*( Q(2) - Q(1) )
C
C      ADUM(N) = 1.
C      BDUM(N) = 1.
C      CDUM(N) = 0.
C      DDUM(N) = 2.*( Q(N) - Q(NM1) )
C
C      CALL TRIDAG( 1, N, ADUM, BDUM, CDUM, DDUM, DQDIZ )
C
C      RETURN
C      END

```

TABLE C-7. Listing of Subroutine ODEINT

SUBROUTINE ODEINT(I, TSTRTO, DTTOT, DTSUG, DTMAX)

SUBROUTINE ***** ODEINT *****

Performs numerical integrations of the system of equations

$D(C(I,K))/DT = GGEN(K) - GDEC(K)$

Where:

T is the independent variable

C(I,K) is the vector of dependent variables (I is fixed during each call to ODEINT)

GGEN(K) is the vector of species generation rates

GDEC(K) is the vector of species destruction rates.

(GDEC(K) is expressed internally as a psuedo first-order relation $GDEC(K) = XI(K)*C(K)$, where XI(K) is the vector of psuedo first-order rate coefficients.

Both GGEN(K) and GDEC(K) are determined by interrogating a user-supplied subroutine, named GEN

TSTRTO is the model time at the begining of the call to odeint

DTTOT is the time interval over which the equations are integrated

DTMAX is the (user specified) maximum allowable time step

DTSUG is the "suggested" initial time step for the integration. If this is set negative by the calling program, then ODEINT will determine its own step size. (After a successful integration, the final step size is passed back in DTSAVE(I). It should be used to establish DTSUG on repeated calls.)

The following parameters affect the mechanics of the numerical integration. They are held in common blocks, and should be initialized in the SETUP subroutine.

TABLE C-7 Continued

```

c      NCORR is the desired number of corrector passes
c      per time step. (**An odd number is recommended**)
c
c      IEXP determines stiff integration method: "asymptotic" (IEXP = 0),
c      or "exponentially assisted" (IEXP = 1)
c
c      CMIN = values of dependent variables, below which
c      they can be considered as insignificant to the
c      overall computation. Must be set as positive,
c      non-zero numbers prior to subroutine call.
c
c      CERROR = values of dependent variables, below which the
c      convergence error criterion is relaxed. Must be set as
c      positive, non-zero numbers prior to subroutine call.
c      Typically, one should set CMIN(I) < .001*CERROR(I).
c
c      EPS = maximum allowable normalized disagreement between the
c      predictor and corrector, or between successive corrector
c      cycles; i. e., maximum convergence error.
c
c      RATESEF = values of psuedo first-order decay coefficient
c      above which the corresponding equations are considered stiff.
c      This parameter can be adjusted to optimize computational
c      efficiency of the algorithm. For typical air chemistry
c      problems, a suggested value is .01 sec(-1).
c
c      DTMIN = minimum allowable step size

```

```

c-----
c      This "PLUVIUS, MOD5.0" version of ODEINT was prepared
c      December, 1983 from an earlier, standard version written
c      by J. M. Hales at Stockholm University in 1983. ODEINT
c      has originated via an extensive modification of the
c      "CHEMEQ" code published by T. R. Young,
c      (NRL Memorandum Report (1980)).
c-----

```

```

      INCLUDE 'PLUVCMN'

```

```

      +  DIMENSION STIFF(NCMAX), FFP(NCMAX), CSTART(NCTMAX),
          GGENP(NCMAX), XI(NCMAX), XIP(NCMAX), PRED(NCMAX)

```

```

      INITIALIZE VARIABLES AND FLAGS

```

TABLE C-7 Continued

```

C      IFLG = TERMINAL INCREMENT FLAG; = 1 WHEN ON LAST
C      TIMESTEP OF INTEGRATION.
C      TN = CURRENT VALUE OF DEPENDENT VARIABLE
C      DTREM = REMAINING SPAN TO BE INTEGRATED
C
      DO K = 1, NTOT
          CNN(K) = C(I,K)
      END DO
      DO K = 1, NCOMP
          CNN(K) = AMAX1( CNN(K), CMIN(K) )
      END DO

      IFLG = 0
      TN = TSTRTO
      TS = TSTRTO
      DTREM = DTTOT
      PFACT = 1.

C
C      DETERMINE INITIAL STEP SIZE: USE "SUGGESTED VALUE"
C      DTSUG IF THIS VALUE IS SUPPLIED AS A POSITIVE
C      NUMBER IN THE SUBROUTINE CALL; OTHERWISE COMPUTE
C      STEP SIZE INTERNALLY.
C
      IF (DTSUG .GT. 0.) THEN
          DTAU = AMIN1(DTSUG, DTTOT)
      ELSE
          CALL GEN(I, 1, TS, DTAU, 1 )
          SCRTCH = 0.
          DO 20 K = 1, NCOMP
              GGEN(K) = GGEN(K)*URATIO(I)
              GDEC(K) = GDEC(K)*URATIO(I)
              DMY1 = .1*EPS*ABS(GGEN(K))-GDEC(K)
              DMY2 = SIGN(1./CNN(K), DMY1)
              DMY1 = DMY2*GDEC(K)
              DMY2 = -ABS(ABS(GGEN(K))-GDEC(K))*DMY2
              DMY1 = AMAX1(DMY1, DMY2)
              SCRTCH = AMAX1(DMY1, SCRTCH, 1.E-20)
          20 CONTINUE
          DTAU = .5/SCRTCH
          DTAU = AMIN1(DTAU, DTMAX)
      ENDIF

```

TABLE C-7 Continued

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C
C      BEGIN AN INTEGRATION STEP FOR STEP-SIZE DTAU
C
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
30      DTREM = DTREM-DTAU
        PFACT = .5*(PFACT+1.)
        NFLAG = 0
C      (NFLAG IS FLAG WHICH IS SET TO 1 WHEN A NEGATIVE
C      VALUE OF THE DEPENDENT VARIABLE IS DETECTED)

C
C      CHECK FOR RUNAWAY COMPUTATION (DTAU .LT. DTMIN)
C
        IF (DTAU .LT. DTMIN) THEN
            WRITE(LUNOUT,2000) I, TS
            STOP 99
        END IF
2000    +   FORMAT(/' *** STEP SIZE BELOW MINIMUM VALUE IN ODEINT ***'/
        ' GRID POINT =', I3/' MODEL TIME =', E12.4 )

C
C      CHECK FOR FINAL SUBINCREMENT IN INTEGRATION.
C      PRESERVE TIMESTEP AND SET FLAG IF FINAL.
C
        IF (DTREM .LE. 0.) THEN
            IFLG = 1
            DTSAVE(I) = DTAU
            DTAU = DTAU+DTREM
            DTREM = 0.
        ENDIF

C
C      SAVE CURRENT VALUES OF DEPENDENT VARIABLES IN CASE
C      STEP HAS TO BE REPEATED
C
        DO 35 K = 1, NTOT
            CSTART(K) = CNN(K)
35      CONTINUE

```

TABLE C-7 Continued

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      PREDICTOR PHASE
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      SET GENERATION AND DECAY RATES
C
C      JPASSO = 1
C      CALL GEN(I, 1, TS, DTAU, JPASSO)
C
C      SET CURRENT TIME
C      CHECK FOR STIFFNESS AND SET FLAGS
C
DO 40 K = 1, NCOMP
  GGEN(K) = GGEN(K)*URATIO(I)
  GDEC(K) = GDEC(K)*URATIO(I)
  GGENP(K) = GGEN(K)
  CSTART(K) = CNN(K)
  XIP(K) = GDEC(K)/CNN(K)
  STIFF(K) = XIP(K)-RATESF(K)
  STIFF(K) = .5+SIGN(.5, STIFF(K))
  FFP(K) = GGEN(K)-GDEC(K)
  IF (IEXP .EQ. 0) THEN
    CNN(K) = DTAU*FFP(K)/(1.+XIP(K)*DTAU*STIFF(K))+CNN(K)
  ELSE
    IF (STIFF(K) .GT. .99) THEN
      DMY1 = XIP(K)*DTAU
      EXP1 = 1.
      IF (DMY1 .LT. 1.E30) EXP1 = 1.-EXP(-DMY1)
      CNN(K) = FFP(K)*EXP1/XIP(K)+CNN(K)
    ELSE
      CNN(K) = FFP(K)*DTAU+CNN(K)
    ENDIF
  ENDIF
  IF (CNN(K) .LT. 0..AND.STIFF(K) .LT. .99) THEN
    NFLAG = 1
    GO TO 92
  ENDIF
  CNN(K) = AMAX1(CNN(K), CMIN(K))-
  PRED(K) = CNN(K)
40 CONTINUE

```

TABLE C-7 Continued

CC

C

C CORRECTOR PHASE

C

CC

ICORR = 1

TS = TN+DTAU

50

JPASSO = JPASSO + 1

CALL GEN(I, 1, TS, DTAU, JPASSO)

DO 60 K = 1, NCOMP

GGEN(K) = GGEN(K)*URATIO(I)

GDEC(K) = GDEC(K)*URATIO(I)

XI(K) = GDEC(K)/CNN(K)

XIM = .5*(XIP(K)+XI(K))

GGENM = .5*(GGEN(K)+GGENP(K))

IF (STIFF(K) .LT. .99) THEN

CNN(K) = CSTART(K)+DTAU*(GGENM-.5*XIM*(CNN(K)+CSTART(K)))

IF (CNN(K) .LT. 0.) THEN

NFLAG = 1

GO TO 92

ENDIF

ELSE IF (IEXP .EQ. 0) THEN

DMY1 = DTAU*(1+.5*XIM*DTAU)

CNN(K) = CSTART(K)+(GGENM-CSTART(K)*XIM)*DMY1/(1.+XIM*DMY1)

ELSE

DMY1 = XIM*DTAU

EXP1 = 1.

IF (DMY1 .LT. 1.E30) EXP1 = 1.-EXP(-DMY1)

CNN(K) = (GGENM/XIM-CSTART(K))*EXP1+CSTART(K)

ENDIF

CNN(K) = AMAX1(CNN(K), CMIN(K))

60

CONTINUE

ICORR = ICORR+1

C

C

REPEAT CORRECTOR PASS NCORR TIMES

C

IF (ICORR .LE. NCORR) GO TO 50

TABLE C-7 Continued

```

CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      ERROR CHECK AND STEP SIZE ADJUSTMENT
C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C
C      BASIC CONVERGENCE CRITERION IS:
C      ABS( (PREDICTOR-CORRECTOR)/CORRECTOR ) _ EPS
C
C      THE CONVERGENCE CRITERION IS RELAXED UNDER A NUMBER OF
C      CIRCUMSTANCES. THIS ERROR RELAXATION SHOULD BE CONSIDERED
C      "APPLICATION-DEPENDENT", AND THE USER MAY WISH TO MODIFY IT
C      AS REQUIRED. IN THE AIR-CHEMISTRY APPLICATIONS OF THE PLUVIUS
C      MOD 5 USERS' MANUAL, ERRORS ARE RELAXED WHENEVER:
C      1) CONCENTRATIONS APPROACH NEGLIGIBLE VALUES (RLOCON)
C      2) THE STARTING CONCENTRATION IS NEGLIGIBLY SMALL (RZRST)
C      3) THE PROJECTED INCREASE IS SO LARGE AS TO MAKE THE CURRENT
C         VALUE AND ITS RELATIVE ERROR SMALL BY COMPARISON (RFASTI)
C      4) THE PROJECTED DECREASE IS RAPID (RFASTD)
C
80      ERRMX = 1.E-6
C      SETTING ERRMX TO 1.E-6 LIMITS STEP SIZE INCREASE TO SQRT(1.E6*EPS)
C
DO 90 K = 1, NCOMP
  RLOCON = 0.5*(CSTART(K) + CNN(K))/CERROR(K)
  RZRST = ABS( CSTART(K)/CMIN(K) - 1. )
  PROJTN = CSTART(K) + DTREM*FFP(K)/(1.+XIP(K)*DTREM*STIFF(K))
  IF (PROJTN .GT. 0.) THEN
    RFASTI = CNN(K)/PROJTN
    RFASTD = PROJTN/CMIN(K)
  ELSE
    RFASTI = 1.
    RFASTD = 0.
  END IF
  REDFTR = AMIN1(1., RLOCON, RFASTD, RFASTI, RZRST)

  ERR = (CNN(K)-PRED(K))/AMAX1(CNN(K),PRED(K))
  ERELAX = ABS(ERR)*REDFTR
  ERRMX = AMAX1(ERELAX, ERRMX)
90  CONTINUE
C
C      ERROR EXCEEDS TOLERANCE. SET PENALTY FACTOR AND SET UP DATA FOR RESTART
C      IF NEGATIVE VALUES WERE EXPERIENCED (NFLAG=1), HALVE THE STEPSIZE.
C      OTHERWISE, COMPUTE NEW STEP SIZE BASED ON SIZE OF ERROR
C
      IF (ERRMX .LT. EPS) GO TO 94

```


TABLE C-7 Continued

```

92      PFACT = 0.5
        TS = TN
        DO K = 1, NTOT
            CNN(K) = CSTART(K)
        END DO
        DTREM = DTREM+DTAU
        IFLG = 0
        IF (NFLAG .EQ. 1) THEN
            DTAU = DTAU/2.
            GO TO 30
        ELSE
            GOTO 96
        ENDIF

C
C      ERROR WAS ACCEPTABLE.
C      RETURN UPON SUCCESSFUL COMPLETION (IFLG=1)
C      OTHERWISE, COMPUTE NEW (EXPANDED) STEP SIZE
C
94      IF (IFLG .EQ. 1) THEN
            DO K = 1, NTOT
                C(I,K) = CNN(K)
            END DO
            RETURN
        ENDIF

C
C      COMPUTE NEW STEP SIZE
C
96      EPSRTO = EPS/ERRMX

C
C      USE NEWTON'S METHOD TO ESTIMATE SQRT(EPSRTO)
        SQRT0 = .5*(EPSRTO+1.)
        DO IDUM = 1, 2
            SQRT0 = .5*(SQRT0+EPSRTO/SQRT0)
        END DO

        DTAU = DTAU*SQRT0*.9*PFACT
        DTAU = AMIN1(DTAU, DTMAX)

C
C      RECYCLE FOR REDUCED STEP SIZE IF ERROR IS TOO HIGH
C      OTHERWISE, ADVANCE INDEPENDENT VARIABLE AND CYCLE TO
C      PREDICTOR PHASE
C
        IF (ERRMX .LE. EPS) TN = TS
        GO TO 30

END

```

TABLE C-8. Listing of Subroutine SETVEC

```

C      SUBROUTINE SETVEC ( K, FXBTC1, FXBTD1, FXTPC1, FXTPD1 )
C
C      CALCULATES, FOR SPECIES K,
C      MASS BALANCE EQUATION COEFFICIENTS C1 AND D1ADV
C      FLUX BOUNDARY CONDITION COEFFICIENTS
C
      INCLUDE 'PLUVCMN'

      DO I = 1, N
        C1(I) = C1DWAP(I) + C1DLCS(I)
        D1ADV(I) = 0.
      END DO

      IF (ITOP(K) .GT. 0) THEN
        FXTPC1 = 2.0*WR(N,K)/DZDIZ(N)
        FXTPD1 = -(FT(K) + FTOLD(K))/DZDIZ(N)
      END IF

      IF (IBOT(K) .GT. 0) THEN
        FXBTC1 = -2.0*WR(1,K)/DZDIZ(1)
        FXBTD1 = (FB(K) + FBOLD(K))/DZDIZ(1)
      END IF

      RETURN
      END

```

TABLE C-9. Listing of Subroutine TEMPF

```

C      SUBROUTINE TEMPF( FXBTC1, FXBTD1, FXTPC1, FXTPD1 )
C
C      TEMPF CALCULATES THE COEFFICIENTS FOR THE ENERGY BALANCE EQUATION
C      AND FOR THE BOUNDARY RELATIONS FOR TEMPERATURE
C
C      IT ALSO CALCULATES ISSAT AND CPCSPS VECTORS WHICH ARE USED IN GEN
C      ISSAT = 1 IF SATURATION AT A GRID POINT
C      0 IF NO SATURATION AT A GRID
C      CPCSPS = (AIR HEAT CAPACITY)*(AIR DENSITY)*(PSI1 FACTOR)
C      [SEE USER'S MANUAL FOR DEF. OF PSI1]
C
C      *** TEMPF SHOULD ALWAYS BE ENABLED (ITEMP=1) IF WAGRID IS NON-ZERO ***
C
C      THIS SUBROUTINE SHOULD NOT BE USED TO SET INITIAL TEMPERATURE
C      AND DENSITY VALUES. THEY SHOULD BE INITIALLY SET IN
C      EITHER 'PRESSF' OR 'SETUP'
C
C      THE 'GEN' SUBROUTINE SHOULD SET
C      GGEN(KTEMP) = HDOTL / CPCSPS(I)
C      HDOTL IS A LATENT HEATING TERM, AND IS DEFINED IN THE PLUVIUS MOD-5
C      USER'S MANUAL. ITS DIMENSIONS ARE (ERG/CM**3/SEC)
C
C
C      INCLUDE 'PLUVCMN'
C
C      DIMENSION GAMMAW(NZMAX), PSI1(NZMAX), GCPSI(NZMAX)
C      EQUIVALENCE (GAMMAW(1), AMAT(1,1,1))
C      EQUIVALENCE (PSI1(1), BMAT(1,1,1))
C      EQUIVALENCE (GCPSI(1), CMAT(1,1,1))
C
C      DATA GAMMAW/-9.76E-5/      ! DRY ADIABATIC LAPSE RATE (DEG K/CM)
C      DATA CP/2.91E8/           ! AIR HEAT CAPACITY, CONSTANT PRESSURE
C                                ! (ERG/MOLE/DEG K)
C      DATA R/8.314E7/           ! GAS CONSTANT (ERG/MOLE/DEG K)
C      DATA HLC/4.5E11/          ! LATENT HEAT OF CONDENSATION (ERG/MOLE WATER)
C
C      DATA CPCSPS/ NZMAX*1.2E4 /      ! TO AVOID DIVIDE BY ZERO IN GEN
C
C
C      DETERMINE SATURATION, AND COMPUTE GAMMAW AND PSI1
C
C      L = LDIF(KTEMP)
C      DO I = 1, N
C        TEMPK = COLD(I,KTEMP)
C        CS(I) = RHOAIR( PRESS(I), TEMPK )

```

TABLE C-9 Continued

```

ISSAT(I) = 0
CPCSPS(I) = CP*CS(I)

C   IFOG=0 TURNS OFF MOISTURE
    IF (IFOG .NE. 0) THEN
        CVAPSAT = SAT( TEMPK )
        DUMMY1 = HLC*CVAPSAT/(CS(I)*R*TEMPK)
        PSI1(I) = 1. + DUMMY1*HLC/(CP*TEMPK)
        PSI2 = 1. + DUMMY1

C   GAMMAW IS MOIST ADIABATIC LAPSE RATE
        GAMMAW(I) = GAMMAD*PSI2/PSI1(I)
        IF (COLD(I,KVAPCL) .GT. CVAPSAT) THEN
            ISSAT(I) = 1
            CPCSPS(I) = CP*CS(I)*PSI1(I)
        END IF
    END IF
END DO

C   FOR DEGENERATE GRID CASE, EXIT HERE
C   IF (N .LE. 3) RETURN

C   CALCULATE C1 AND D1ADV
C   DO I = 1, N
        C1(I) = C1DWAP(I)
        IF (ISSAT(I) .EQ. 0) THEN
            GCPSI(I) = CPCSPS(I)*GAMMAD
            D1ADV(I) = (WAGRID(I) + WAP(I))*GAMMAD
        ELSE
            GCPSI(I) = CPCSPS(I)*GAMMAW(I)
            D1ADV(I) = (WAGRID(I) + WAP(I))*GAMMAW(I)
        END IF
    END DO

    DGCPS = D(1,L) * 0.5 * (GCPSI(1)+GCPSI(2))
    D1ADV(1) = D1ADV(1) - 2.*DGCPS/(CPCSPS(1)*DZDIZ(1))
    FXBTD1 = (FB(KTEMP) + FBOLD(KTEMP))/(CPCSPS(1)*DZDIZ(1))
    FXBTC1 = 0.0

```

TABLE C-9 Continued

```

DO I = 2, NM1
  DGCPS0 = DGCPS
  DGCPS = D(I,L) * 0.5 * (GCPSI(I)+GCPSI(I+1))
  D1ADV(I) = D1ADV(I) - (DGCPS - DGCPS0)/(CPCSPS(I)*DZDIZ(I))
END DO

D1ADV(N) = D1ADV(N) + 2.*DGCPS/(CPCSPS(N)*DZDIZ(N))
FXTPD1 = - (FT(KTEMP) + FTOLD(KTEMP))/(CPCSPS(N)*DZDIZ(N))
FXTPC1 = 0.0

```

C
C
C

CALCULATE ADIFFU, BDIFFU, AND CDIFFU (SIMILAR TO CODE IN DERIV)

```

DUMOLD = 0.
DO I = 1, NM1
  CSPSDZ = CPCSPS(I)*DZDIZ(I)
  DUM = D(I,L) * 0.5 * (CPCSPS(I+1)+CPCSPS(I)) / (Z(I+1)-Z(I))

  ADIFFU(I,L) = DUMOLD/CSPSDZ
  CDIFFU(I,L) = DUM/CSPSDZ
  BDIFFU(I,L) = -( ADIFFU(I,L) + CDIFFU(I,L) )

  DUMOLD = DUM
END DO

ADIFFU(N,L) = 2.*DUMOLD/(CPCSPS(N)*DZDIZ(N))
BDIFFU(N,L) = -ADIFFU(N,L)
CDIFFU(N,L) = 0.

CDIFFU(1,L) = 2.*CDIFFU(1,L)
BDIFFU(1,L) = -CDIFFU(1,L)

RETURN
END

```

TABLE C-10. Listing of Subroutine TRIDG2

```

SUBROUTINE TRIDG2( JLO, JHI, AMAT, BMAT, CMAT, DVEC, UVEC )
C
C ROUTINE FOR SOLVING A SYSTEM OF PAIRED SIMULTANEOUS LINEAR EQUATIONS WITH
C   A TRIDIAGONAL COEFFICIENT MATRIX USING THOMAS'S ALGORITHM
C   IN THIS CASE, EACH UNKNOWN IS A 2 ELEMENT VECTOR, AND EACH ELEMENT OF
C   COEFFICIENT MATRIX IS ITSELF A 2 BY 2 MATRIX
C
C INPUTS:
C   AMAT - AMAT(I) IS THE SUB-DIAGONAL ELEMENT OF ROW I OF THE
C           COEFFICIENT MATRIX
C   BMAT - BMAT(I) IS THE DIAGONAL ELEMENT OF ROW I OF THE
C           COEFFICIENT MATRIX
C   CMAT - CMAT(I) IS THE SUPER-DIAGONAL ELEMENT OF ROW I OF THE
C           COEFFICIENT MATRIX
C   DVEC - DVEC(I) IS THE RIGHT-HAND SIDE ELEMENT OF THE I-TH EQUATION
C
C   JLO, JHI - ONLY THE EQUATIONS NUMBERED JLO THRU JHI INCLUSIVE ARE
C               SOLVED (I.E., ROWS JLO THRU JHI OF THE MATRIX)
C
C OUTPUT:
C   UVEC - UVEC(I) IS THE I-TH ELEMENT OF THE SOLUTION VECTOR
C
C ROUTINE DOES NOT CHECK THAT SYSTEM IS NON-SINGULAR, SO WILL FAIL
C   (DIVIDE BY ZERO) IF IT IS
C
C   DIMENSION AMAT(2,2,JHI), BMAT(2,2,JHI), CMAT(2,2,JHI)
C   DIMENSION DVEC(2,JHI), UVEC(2,JHI)
C
C   DIMENSION XMAT(2,2), YMAT(2,2), ZMAT(2,2), XVEC(2), YVEC(2)
C
C FORWARD PASS - REDUCE THE SYSTEM BY ELIMINATING THE SUB-DIAGONAL ELEMENTS.
C   IN THE REDUCED SYSTEM,
C       THE NEW DIAGONAL ELEMENTS ARE UNITY
C       THE NEW SUPER-DIAGONAL ELEMENTS ARE IN AMAT (WHOSE CONTENTS
C           ARE THUS DESTROYED)
C       THE NEW RIGHT-HAND SIDE IS IN DVEC (THUS DESTROYED ALSO)
C   IF IT IS DESIRED NOT TO DESTROY THE AMAT AND DVEC ELEMENTS,
C       THE ROUTINE CAN BE WRITTEN USING TWO ADDITIONAL WORKING
C       ARRAYS: EMAT(2,2,JHI) AND FVEC(2,JHI)
C
C   DO J = JLO, JHI
C       JM = J-1
C       IF (J.EQ.JLO) THEN
C           XMAT(1,1) = 0.
C           XMAT(1,2) = 0.
C           XMAT(2,1) = 0.
C           XMAT(2,2) = 0.
C           XVEC(1) = 0.
C           XVEC(2) = 0.

```

TABLE C-10 Continued

```

ELSE
  2   XMAT(1,1) = AMAT(1,1,J)*AMAT(1,1,JM) +
      AMAT(1,2,J)*AMAT(2,1,JM)
  2   XMAT(1,2) = AMAT(1,1,J)*AMAT(1,2,JM) +
      AMAT(1,2,J)*AMAT(2,2,JM)
  2   XMAT(2,1) = AMAT(2,1,J)*AMAT(1,1,JM) +
      AMAT(2,2,J)*AMAT(2,1,JM)
  2   XMAT(2,2) = AMAT(2,1,J)*AMAT(1,2,JM) +
      AMAT(2,2,J)*AMAT(2,2,JM)
  2   XVEC(1) = AMAT(1,1,J)*DVEC(1,JM) +
      AMAT(1,2,J)*DVEC(2,JM)
  2   XVEC(2) = AMAT(2,1,J)*DVEC(1,JM) +
      AMAT(2,2,J)*DVEC(2,JM)
END IF

YMAT(1,1) = BMAT(1,1,J) - XMAT(1,1)
YMAT(1,2) = BMAT(1,2,J) - XMAT(1,2)
YMAT(2,1) = BMAT(2,1,J) - XMAT(2,1)
YMAT(2,2) = BMAT(2,2,J) - XMAT(2,2)

DET = YMAT(1,1)*YMAT(2,2) - YMAT(1,2)*YMAT(2,1)
ZMAT(1,1) = YMAT(2,2)/DET
ZMAT(1,2) = -YMAT(1,2)/DET
ZMAT(2,1) = -YMAT(2,1)/DET
ZMAT(2,2) = YMAT(1,1)/DET
C   ZMAT IS INVERSE OF YMAT = BMAT(J) - AMAT(J)*AMAT(J-1)

AMAT(1,1,J) = ZMAT(1,1)*CMAT(1,1,J) + ZMAT(1,2)*CMAT(2,1,J)
AMAT(1,2,J) = ZMAT(1,1)*CMAT(1,2,J) + ZMAT(1,2)*CMAT(2,2,J)
AMAT(2,1,J) = ZMAT(2,1)*CMAT(1,1,J) + ZMAT(2,2)*CMAT(2,1,J)
AMAT(2,2,J) = ZMAT(2,1)*CMAT(1,2,J) + ZMAT(2,2)*CMAT(2,2,J)

YVEC(1) = DVEC(1,J) - XVEC(1)
YVEC(2) = DVEC(2,J) - XVEC(2)

DVEC(1,J) = ZMAT(1,1)*YVEC(1) + ZMAT(1,2)*YVEC(2)
DVEC(2,J) = ZMAT(2,1)*YVEC(1) + ZMAT(2,2)*YVEC(2)
END DO

C
C   BACKWARD PASS - COMPUTE SOLUTION BY BACKWARDS SUBSTITUTION
C
UVEC(1,JHI) = DVEC(1,JHI)
UVEC(2,JHI) = DVEC(2,JHI)
JLOP = JLO+1
DO J2 = JLOP, JHI

```

TABLE C-11. Listing of Subroutine TRIDAG

```

C      SUBROUTINE TRIDAG ( JLO, JHI, AA, BB, CC, DD, VV )
C
C      ROUTINE FOR SOLVING A SYSTEM OF SIMULTANEOUS LINEAR EQUATIONS WITH
C      A TRIDIAGONAL COEFFICIENT MATRIX USING THOMAS'S ALGORITHM
C
C      INPUTS:
C      AA - AA(I) IS THE SUB-DIAGONAL ELEMENT OF ROW I OF THE COEFFICIENT
C      MATRIX
C      BB - BB(I) IS THE DIAGONAL ELEMENT OF ROW I OF THE COEFFICIENT MATRIX
C      CC - CC(I) IS THE SUPER-DIAGONAL ELEMENT OF ROW I OF THE COEFFICIENT
C      MATRIX
C      DD - DD(I) IS THE RIGHT-HAND SIDE ELEMENT OF THE I-TH EQUATION
C
C      JLO, JHI - ONLY THE EQUATIONS NUMBERED JLO THRU JHI INCLUSIVE ARE
C      SOLVED (I.E., ROWS JLO THRU JHI OF THE MATRIX)
C
C      OUTPUT:
C      VV - VV(I) IS THE I-TH ELEMENT OF THE SOLUTION VECTOR
C
C      ROUTINE DOES NOT CHECK THAT SYSTEM IS NON-SINGULAR, SO WILL FAIL
C      (DIVIDE BY ZERO) IF IT IS
C      RIGHT-HAND-SIDE VECTOR ( DD ) IS DESTROYED
C
C      DIMENSION AA(JHI), BB(JHI), CC(JHI), DD(JHI), VV(JHI)
C
C      FORWARD PASS - ELIMINATE SUB-DIAGONAL ELEMENTS AND NORMALIZE
C      DIAGONAL ELEMENTS
C      NEW SUPER-DIAGONAL ELEMENTS HELD IN VV
C      NEW RIGHT-HAND-SIDE ELEMENTS HELD IN DD
C
C      DD(JLO) = DD(JLO)/BB(JLO)
C      BETA = BB(JLO)
C      JLOP1 = JLO+1
C      DO I = JLOP1, JHI
C          VV(I-1) = CC(I-1)/BETA
C          BETA = BB(I) - AA(I)*VV(I-1)
C          DD(I) = (DD(I) - AA(I)*DD(I-1))/BETA
C      END DO
C
C      BACKWARD PASS - SOLVE BY REVERSE SUBSTITUTION
C
C      VV(JHI) = DD(JHI)
C      DO IDUM = JLOP1, JHI
C          I = JHI + JLO - IDUM
C          VV(I) = DD(I) - VV(I)*VV(I+1)
C      END DO
C
C      RETURN
C      END

```


TABLE C-10 Continued

```
J = JHI+JLO-J2
JP = J+1

      UVEC(1,J) = DVEC(1,J) - AMAT(1,1,J)*UVEC(1,JP) -
2      AMAT(1,2,J)*UVEC(2,JP)
      UVEC(2,J) = DVEC(2,J) - AMAT(2,1,J)*UVEC(1,JP) -
2      AMAT(2,2,J)*UVEC(2,JP)
      END DO

      RETURN
      END
```

TABLE C-12. Listing of Subroutine ZERODM

```

SUBROUTINE ZERODM( INITBB )
C
C WHEN THE NUMBER OF GRID POINTS, N, IS SPECIFIED AS 1 OR 2,
C THE NORMAL ADVECTION-DIFFUSION INTEGRATION IS NOT PERFORMED
C RATHER, PLUVIUS PERFORMS AS A SIMPLE PARCEL (OR 2 PARCEL)
C MODEL. THE PURPOSE OF THIS IS TO ALLOW TESTING OF THE CHEMISTRY
C AND INTER-PHASE TRANSFER PORTIONS OF THE CODE IN AN ECONOMICAL
C FASHION.
C
C ZERODM CALCULATES TWO CHANGES WHICH WOULD OCCUR FROM LIFTING THE
C PARCEL AT A VELOCITY OF WAGRID(1). THESE ARE:
C 1. TEMP. IS COOLED AT THE DRY OR MOIST ADIABATIC LAPSE RATE
C 2. CONCENTRATIONS ARE REDUCED IN PROPORTION TO THE REDUCTION
C IN AIR DENSITY
C IF WAGRID(1) IS ZERO, OR IF BOTH ITEMP AND IPRESS ARE ZERO,
C THEN ZERODM DOES NOTHING
C
C INCLUDE 'PLUVCMN'
C
C DIMENSION CSZOLD(2)
C DATA INITZD / 0 /
C
C SAVE DENSITIES ON VERY FIRST ENTRY
C IF ( INITBB .EQ. 1) THEN
C   DO I = 1, N
C     CSZOLD(I) = CS(I)
C   END DO
C END IF
C
C CALC HEIGHT CHANGE
C DZUR = DT*URATIO(1)*WAGRID(1)
C IF ((DZUR.EQ.0.) .AND. (ITEMP.EQ.0)) RETURN
C
C CALC NEW TEMPERATURES
C IF (ITEMP .NE. 0) THEN
C   CALL TEMPF( DUMMY1, DUMMY1, DUMMY1, DUMMY1 )
C   DO I = 1, N
C     C(I,KTEMP) = COLD(I,KTEMP) + DZUR*RLAPSE(
C + COLD(I,KTEMP), CS(I), ISSAT(I) )
C   END DO
C ELSE
C   DO I = 1, N
C     C(I,KTEMP) = COLD(I,KTEMP)
C   END DO
C END IF
C
C NEW PRESSURE
C IF (IPRESS .NE. 0) CALL PRESSF( INITZD )

```

TABLE C-12 Continued

```
C  NEW DENSITIES, AND CHANGES TO SPECIES CONCENTRATIONS
    DO I = 1, N
      CS(I) = RHOAIR( PRESS(I), C(I,KTEMP) )
      RATIOCS = CS(I)/CSZOLD(I)
      DO K = 1, NCOMP
        IF (K .NE. KTEMP) C(I,K) = RATIOCS*COLD(I,K)
      END DO
      CSZOLD(I) = CS(I)
    END DO

    RETURN
  END
```

TABLE C-13. Listing of Subroutine PRESSF

```

C      SUBROUTINE PRESSF( INIT )
C
C      CALCULATES PRESSURE BY INTEGRATING THE HYDROSTATIC EQUATION
C      *** PRESSF SHOULD ALWAYS BE ENABLED (IPRESS=1) IF WAGRID IS NON-ZERO
C
C      WHEN WAGRID(1) IS NOT ZERO, THEN PRESS(1) - THE PRESSURE AT THE
C      BOTTOM OF THE GRID, MUST ALSO BE CALCULATED.  IN THIS VERSION,
C      THIS IS DONE BY INTEGRATING HYDROSTATIC EQN. OVER GRID HEIGHT
C      CHANGE (GLEVL - GLEVLOLD)
C
C      NOTE:  PRESSURE UNITS = DYNES/CM**2
C      AIR DENSITY UNITS = MOLES/CM**3
C
C      INCLUDE 'PLUVCMN'
C
C
C      SET PRESSURE AT BOTTOM GRID
C
C      IF (INIT.EQ.1) THEN
C        PRESS(1) = PRESSØ
C      ELSE
C        DZDUM = GLEVL - GLEVLOLD
C        PRESS(1) = PRESS(1)*EXP(-3.416E-4*DZDUM/C(1,KTEMP))
C      END IF
C      GLEVLOLD = GLEVL
C      CS(1) = RHOAIR(PRESS(1), C(1,KTEMP))
C
C      INTEGRATE HYDROSTATIC EQUATION
C      D(LN(P))/DZ = -G/(R*T)
C
C      DO 1ØØØ I = 2,N
C        DZDUM = Z(I)-Z(I-1)
C        TEMPBB = .5*(C(I-1,KTEMP) + C(I,KTEMP))
C        PRESS(I) = PRESS(I-1)*EXP(-3.416E-4*DZDUM/TEMPBB)
C        CS(I) = RHOAIR( PRESS(I), C(I,KTEMP))
1ØØØ  CONTINUE
C      RETURN
C      END

```

TABLE C-14. Listing of Function RHOAIR

```

FUNCTION RHOAIR( P, TEMPK )
C
C RHOAIR = AIR DENSITY (MOLES/CC)
C P      = PRESSURE (DYNES/CM**2)
C TEMPK  = TEMPERATURE (K)
C
C RHOAIR = P/(8.3144E7*TEMPK)
C RETURN
C END

```

TABLE C-15. Listing of Function RLAPSE

```

FUNCTION RLAPSE ( TEMPK, RHOA, JFOG )
C
C RLAPSE = LAPSE RATE (1/CM)
C ADIABATIC IF JFOG=0
C PSEUDOADIABATIC OTHERWISE
C TEMPK = TEMP (K)
C RHOA = AIR DENSITY (MOLES/CC)
C
C THERMODYNAMIC UNITS ARE CGS (CONSTANTS USE MOLES)
C THE SAT FUNCTION MUST RETURN THE SATURATION VAPOR
C DENSITY (MOLES/CC) AT TEMP TEMPK
C
C DATA GAMMAD/-9.76E-5/ ! DRY ADIABATIC LAPSE RATE (DEG K/CM)
C DATA CP/2.91E8/ ! AIR HEAT CAPACITY, CONSTANT PRESSURE
C ! (ERG/MOLE/DEG K)
C DATA R/8.314E7/ ! GAS CONSTATN (ERG/MOLE/DEG K)
C DATA HLC/4.5E11/ ! LATENT HEAT OF CONDENSATION (ERG/MOLE WATER)
C
C RLAPSE = GAMMAD
C IF (JFOG.NE.0) THEN
C DUMMY1 = HLC*SAT(TEMPK)/(RHOA*R*TEMPK)
C RLAPSE = GAMMAD*(1. + DUMMY1)/(1. + DUMMY1*HLC/(CP*TEMPK))
C END IF
C
C RETURN
C END

```

TABLE C-16. Listing of Function SAT

FUNCTION SAT (TEMPK)

C
C
C
C
C

ROUTINE FOR CALCULATING THE SATURATION CONCENTRATION OF
WATER VAPOR (GRAM-MOLES/CC) AT TEMPK DEGREES KELVIN
(ESAT IS SATURATION VAPOR PRESSURE IN MB)

TEMPC = TEMPK-273.15

ESAT= 6.107799961 + TEMPC*(4.436518521E-1 + TEMPC*(1.428945805E-2

+ + TEMPC*(2.650648471E-4 + TEMPC*(3.031240396E-6

+ + TEMPC*(2.034080948E-8 + TEMPC*6.136820929E-11))))

SAT = (ESAT*1.E3)/(8.3144E7*TEMPK)

RETURN

END

TABLE C-17. Listing of Subroutine COLLECT

```

SUBROUTINE COLLECT ( INIT, ITCOLL, DTCOLL )
C
C ROUTINE DOES OUTPUT TO DISK FILE FOR POST-PROCESSING
C   PARAMETERS ARE OUTPUT AT TIME INTERVALS = DTCOLL
C
C   ITCOLL > 0 - MODEL OUTPUT IS TIME AVERAGED OVER THE INTERVAL
C   ITCOLL < 0 - NO AVERAGING
C
C FOR ITCOLL > 0, INITIAL CONCENTRATION FIELD IS OUTPUT, THEN
C   FIRST SMOOTHED OUTPUT IS FROM (TSTART + .5*DTCOLL) TO
C   (TSTART + 1.5*DTCOLL)
C
C ROUTINE WILL NOT FUNCTION UNLESS DTCOLL > 1.E-5
C
C   INCLUDE 'PLUVCMN'
C
C   PARAMETER (LUNCOL = 8)
C   PARAMETER (NCSUMMX = NZMAX*NCTMAX)
C
C   DIMENSION CSUM(NZMAX, NCTMAX)
C   DATA DTSUM, IEND / 0., 0 /
C   DATA CSUM / NCSUMMX*0. /
C
C   IF (DTCOLL.LE.1.E-5) RETURN
C
C INITIAL ENTRY - WRITE "HEADING" INFO. TO FILE
C
C   IF (INIT .EQ. 1) THEN
C     WRITE(LUNCOL) N, NTOT+2, DTCOLL
C     WRITE(LUNCOL) (Z(I), I=1,N)
C     WRITE(LUNCOL) MTITLE
C     WRITE(LUNCOL) ((NAME(I,K), I=1,5), K=1,NTOT+2)
C     WRITE(LUNCOL) TCLOCK, ((C(I,K),I=1,N),K=1,NTOT),
+      (PRESS(I),I=1,N), (CS(I),I=1,N), GLEVL
C     IF (ITCOLL .GT. 0) THEN
C       TAVEAA = TCLOCK + .5*DTCOLL
C       TAVEZZ = TAVEAA + DTCOLL
C       TCONTZ = TAVEAA
C     ELSE
C       TAVEZZ = DTCOLL - .01*DT
C     END IF
C     RETURN
C   END IF
C
C NORMAL ENTRY - NO AVERAGING

```

TABLE C-17 Continued

```

C      IF (ITCOLL .LT. 0) THEN
          IF (TCLOCK .GE. TAVEZZ) THEN
              WRITE(LUNCOL) TCLOCK, ((C(I,K),I=1,N),K=1,NTOT),
+              (PRESS(I),I=1,N), (CS(I),I=1,N), GLEVL
              TAVEZZ = TAVEZZ + DTCOLL
          END IF
          RETURN
      END IF

C
C      NORMAL ENTRY - AVERAGING
C

C      CHECK FOR END OF RUN
      IF (INIT .EQ. -1) THEN
          IEND = 1
          GO TO 4000
      END IF

      TCLKAA = TCLOCK - DT
      TCLKZZ = TCLOCK + DT
1000  IF (TCLKZZ .LE. TAVEAA) RETURN
      IF (TCLKAA .GT. TAVEZZ) GOTO 4000

C
C      ADD CONTRIBUTION OF CURRENT VALUES TO "RUNNING SUM" IN CSUM
C
      IF (TCLKAA .GT. TAVEAA) THEN
          TCONTA = TCLKAA
      ELSE
          TCONTA = TAVEAA
      END IF
      IF (TCLKZZ .LT. TAVEZZ) THEN
          TCONTZ = TCLKZZ
      ELSE
          TCONTZ = TAVEZZ
      END IF
      DTCONT = TCONTZ - TCONTA
      DTSUM = DTSUM + DTCONT
      DO K = 1, NTOT
          DO I = 1, N
              CSUM(I,K) = CSUM(I,K) + DTCONT*C(I,K)
          END DO
      END DO

C
C      CHECK IF AVERAGING COMPLETE OVER PRESENT INTERVAL (TAVEAA TO TAVEZZ)
C      IF NOT, RETURN.  OTHERWISE, OUTPUT AVERAGED VALUES

```


TABLE C-17 Continued

```

C      IF (TCLKZZ .LT. TAVEZZ) RETURN

4000  IF (DTSUM .LE. 1.E-5) RETURN
      DO K = 1, NTOT
        DO I = 1, N
          CSUM(I,K) = CSUM(I,K)/DTSUM
        END DO
      END DO
      TOUT = .5*(TAVEAA + TCONTZ)
      WRITE(LUNCOL) TOUT, ((CSUM(I,K),I=1,N),K=1,NTOT),
+      (PRESS(I),I=1,N), (CS(I),I=1,N), GLEVL
      IF (IEND .EQ. 1) RETURN

C
C      NOW PREPARE FOR NEW AVERAGING INTERVAL
C
      TAVEAA = TAVEZZ
      TAVEZZ = TAVEZZ + DTCOLL
      TCONTZ = TAVEAA
      DTSUM = 0.
      DO K = 1, NTOT
        DO I = 1, N
          CSUM(I,K) = 0.
        END DO
      END DO
      GO TO 1000

END

```

TABLE C-18. Listing of Subroutine PRINT

```

SUBROUTINE PRINT( INIT, TSTART, TSTOP, NPRINT, DTPRIN, DTCOLL )
C
C HANDLES PRINTED OUTPUT
C OUTPUT GOES TO UNIT LUNOUT
C

      INCLUDE 'PLUVCMN'
      COMMON/FILTERCMN/ NFILTR, FILFAC(NCMAX), MAXITA, MAXITB,
+       NFSRCH, NFSET
      DIMENSION CDUM(NNAMMX), NAMEBC(4,3)

      DATA NAMEBC/ 'FL', 'UX', ' ', ' ', ' ', 'CO', 'NC', ' ', ' ', ' ',
+       'OU', 'TF', 'LO', 'W ' /

      IF (INIT .EQ. 0) GO TO 20000

C
C
C INITIAL CALL - PRINT RUN HEADING INFORMATION
C
C

      WRITE(LUNOUT,9100) MTITLE
      DO K = 1, NCOMP
        IF (ITOP(K) .GT. 0) THEN
          JT = 1
        ELSE
          JT = 2
        END IF
        IF (IBOT(K) .GT. 0) THEN
          JB = 1
        ELSE IF (IBOT(K) .EQ. 0) THEN
          JB = 2
        ELSE
          JB = 3
        END IF
        IF (MOD(K,5) .EQ. 1) WRITE(LUNOUT,9110)
        WRITE(LUNOUT,9110) K, (NAME(L1,K),L1=1,5),
+       (NAMEBC(L2,JT),L2=1,4),
+       (NAMEBC(L3,JB),L3=1,4), LDIF(K), FILFAC(K)
      END DO
      IF (NCNSTR .GT. 0) THEN
        WRITE(LUNOUT,9120)
        DO KDUM = 1, NCNSTR
          K = KDUM + NCOMP
          IF (MOD(KDUM,5) .EQ. 1) WRITE(LUNOUT,9110)
          WRITE(LUNOUT,9110) K, (NAME(L1,K),L1=1,5)
        END DO
      END IF

```

TABLE C-18 Continued

```

WRITE(LUNOUT,9130) IGEN, IPRESS, IVERT, IDIFF, ISETTL,
+   IFOG, ITEMP, IBOUND, ISHEAR
WRITE(LUNOUT,9140) TSTART, TSTART/3600., NPRINT,
+   TSTOP, TSTOP/3600., DTPRIN, DTCOLL
WRITE(LUNOUT,9150)

1500   NCA=NTOT+1
      NCB=NTOT+2
      DO 1600 K = NCA,NCB
1600   DO 1600 LL = 2,5
      NAME(LL,K) = 2H
      NAME(1,NCA) = 2HP
      NAME(1,NCB) = 2HCS

      NPERPG=11
      NPAGE=1+(NCB-1)/NPERPG

C
C
C   AFTER INITIAL CALL
C
C
2000   CONTINUE
      DO 4000 IPAGE=1,NPAGE
        KLO=(IPAGE-1)*NPERPG+1
        KHI=MIN0(NCB,IPAGE*NPERPG)
        IF ((IPAGE.EQ.1) .OR. (N.GT.2)) THEN
          WRITE(LUNOUT,9000) TCLOCK, TCLOCK/3600., GLEVL*1.E-5
          WRITE(LUNOUT,9001) DT,WAGRID(1)
        ELSE
          WRITE(LUNOUT,9003)
        END IF
        WRITE(LUNOUT,9005) ((NAME(LL,K),LL=1,5),K=KLO,KHI)
        WRITE(LUNOUT,9006)
        DO IREV=1,N
          I=N+1-IREV
          ZDUM=(Z(I)+GLEVL)*1.E-5
          DO K = KLO, KHI
            IF (K .LE. NTOT) THEN
              CDUM(K) = C(I,K)
            ELSE IF (K .EQ. NCA) THEN
              CDUM(K) = PRESS(I)
            ELSE
              CDUM(K) = CS(I)
            END IF
          END DO
          IF (MOD(I,5).EQ.0) WRITE(LUNOUT,9010)
          WRITE(LUNOUT,9010) ZDUM,(CDUM(K),K=KLO,KHI)
        END DO
      END DO

```

TABLE C-18 Continued

```

      END DO
4000  CONTINUE
      RETURN

9000  FORMAT(1H1, 'TCLOCK', F10.2, '      (' , F7.3, ' HRS)',
2      20X, 'GLEVL (KM)', F7.3 )
9003  FORMAT(1X)
9001  FORMAT(' DT', F14.2, 38X, 'WAGRID(1)', F11.2 )
9005  FORMAT(/1X, ' Z(KM)', 11(1X, 5A2))
9006  FORMAT(1H )
9010  FORMAT(1X, F6.3, 11E11.4)

9100  FORMAT( 1H1/
+      9X, '++++++' /
+      9X, '+' /
+      9X, '+ PLUVIUS REACTIVE STORM MODEL (MOD 5.0) ' /
+      9X, '+' /
+      9X, '++++++' /
+      // 1X, 'RUN ID: ', 40A2 ///
+      1X, 'COMPUTED SPECIES', 5X, 'TOP B.C.', 5X, 'BOTTOM B.C.',
+      5X, 'DIFFUS. REGIME', 5X, 'FILTER FACT.' )
9110  FORMAT( 1X, I3, 3X, 5A2, 6X, 4A2, 6X, 4A2, 6X, I8, 12X, F7.2 )
9120  FORMAT(/1X, 'CONSTRAINED SPECIES' )
9130  FORMAT(/////1X, 'CONTROL DATA'///
+      1X, 'IGEN ', I3, 10X, 'IPRESS', I3, 10X, 'IVERT ', I3 /
+      1X, 'IDIFF ', I3, 10X, 'ISETTL', I3, 10X, 'IFOG ', I3 /
+      1X, 'ITEMP ', I3, 10X, 'IBOUND', I3, 10X, 'ISHEAR', I3 )
9140  FORMAT(/1X, 'TSTART', F9.1, ' (' , F6.2, ' HRS)',
+      15X, 'NPRINT', I11 /
+      1X, 'TSTOP ', F9.1, ' (' , F6.2, ' HRS)',
+      15X, 'DTPRIN', F11.1 / 45X, 'DTCOLL', F11.1 )
9150  FORMAT(/1X, 'UNITS USED IN PLUVIUS ARE CGS:' /
+      5X, 'TIME SEC' /
+      5X, 'HEIGHT CM' /
+      5X, 'VELOCITY CM/SEC' /
+      5X, 'TEMPERATURE DEG K' /
+      5X, 'MASS GM' /
+      5X, 'PRESSURE DYNES/CM**2' /
+      5X, 'ENERGY ERGS' /
+      5X, 'CONCENTRATION GM MOLE/CM**3' /
+      10X, '(NOTE: THIS IS',
+      ' CONCENTRATION PER VOLUME OF TOTAL SPACE (AIR),' /
+      17X, 'NOT CONCENTRATION PER VOLUME OF LIQUID) ' /
+      1X, 'ALL OUTPUT IN THESE UNITS UNLESS OTHERWISE NOTED')

```

END

Table C-19 provides a description of PLUVIUS variables and parameters which the user may have occasion to use, and all global variables (regardless of utility). This table does not include all of the internal variables used in the code, nor does it include variables from the Class I subroutines of Examples 1 and 2. These variables are either self-documented within the code listings or described in Sections 4 and 5, respectively.

Arrays are shown in the table with appropriate index variables. The index variable I refers to vertical grid position; K refers to species number; and L refers to diffusion regime. J1 and J2 refer to "other" indices; most arrays shown with these indices are used in the solution of the advection-diffusion component and should not be of interest to the user. Where appropriate, physical units for variables are shown in brackets [].

TABLE C-19. Description of PLUVIUS Variables and Parameters

<u>Variable</u>	<u>Description</u>
ADIFFU (I,L)	ADIFF in Eq. (A9). [sec^{-1}]
AMAT (J1,J2,I)	AM in Eqs. (A12) and (A13).
BDIFFU (I,L)	BDIFF in Eq. (A9). [sec^{-1}]
BMAT (J1,J2,L)	BM in Eqs. (A12) and (A14).
C (I,K)	Dependent variable values (i.e., temperature or species concentration). [K or mole/cc]
CB (K)	Dependent variable value at bottom boundary; C_B in Eq. (16) or T_B in Eq. (41).
CDIFFU (I,L)	CDIFF in Eq. (A9). [sec^{-1}]
CERROR (K)	Values of dependent variables, below which the convergence error criterion is relaxed during integration of the generation components (see Appendix B). [mole/cc or K]

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
CMAT (J1,J2,I)	CM in Eqs. (A12) and (A15).
CMIN (K)	Values of dependent variables, below which they can be considered as insignificant to the overall computation (see Appendix B). [mole/cc or K]
CNN (K)	Working array to hold C(I,K) values at a particular grid I during integration of generation component of mass-balance equations (used in subroutines ODEINT and GEN). [mole/cc or K]
COLD (I,K)	Working array to hold previous C(I,K) values during advection-diffusion integration. [K or mole/cc]
CPCSPS (I)	$(c \cdot \chi C_p)$ in Eqs. (34)-(36). [erg/cc·K]
CS (I)	Air density. [mole/cc]
CT (K)	Dependent variable value at top boundary; $\hat{C}_T$ in Eq. (15) or $\hat{T}_T$ in Eq. (40). [mole/cc or K]
C1 (I)	C1 in Eq. (A10). [sec^{-1}]
C1DLCS (I)	Second term in right-hand side of Eq. (A10). [sec^{-1}]
C1DWAP (I)	First term in right-hand side of Eq. (A10). [sec^{-1}]
D (I,L)	Eddy diffusivity. [cm^2/sec]
DT	Current time-step for advection-diffusion integration. [sec]
DTAU	Current integration time-step in subroutine ODEINT. Passed as parameter to subroutine GEN. [sec]
DTCOLL	Time interval for output of model results to mass storage. [sec]
DTMAX	Parameter passed to subroutine ODEINT, specifying maximum time-step for integration of generation components. [sec]

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
FT (K)	Vertical flux at top boundary; $\hat{f}_T$ in Eq. (17) or $\hat{q}_T$ in Eq. (38). [mole/cm ² sec or erg/cm ² sec]
FTOLD (K)	Previous value of FT(K). During an advection-diffusion integration step, FT refers to time TNEXT and FTOLD refers to time TCLOCK.
FXBTC1	The term $\frac{-2w_r1}{\Delta z_1}$ in Eq. (A28), or similar term for temperature case.
FXBTD1	The term $\frac{1}{\Delta z_1} (\hat{f}_B^j + \hat{f}_B^{j+1})$ in Eq. (A30), or similar term for temperature case.
FXTPC1	The term $\frac{2w_{rn}}{\Delta z_n}$ in Eq. (A35), or similar term for temperature case.
FXTPD1	The term $-\frac{1}{\Delta z_n} (\hat{f}_T^j + \hat{f}_T^{j+1})$ in Eq. (A36), or similar term for temperature case.
GDEC (K)	Decay rates [loss or sink terms in right-hand side of Eq. (43) or (45)]. [mole/cc·sec or K/sec]
GGEN (K)	Generation rates [source terms in right-hand side of Eq. (43) or (45)]. [mole/cc·sec or K/sec]
GLEVL	Changing component of grid height. Total grid height = Z(I) + GLEVL. [cm]
I	Index variable used to specify vertical grid number.
IBOT (K)	Bottom boundary condition designator for computed species: positive → flux specified, zero → concentration specified, negative → out-flow specified.
IBOUND	Bypass control variable for boundary conditions (see Section 3).

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
IDIFF	Bypass control variable for eddy diffusivity (see Section 3).
IEXP	Flag specifying stiff integration method in subroutine ODEINT (see Appendix B).
IFOG	Bypass control variable for water condensation (see Section 3).
IGCALC	Parameter passed to subroutine GEN, specifying either that only constrained variables need be calculated (IGCALC = 0), or that GGEN and GDEC are also required (IGCALC = 1).
IGEN	Bypass control variable for physico-chemical transformation (see Section 3).
INIT	Initialization flag. INIT = 1 during initialization. INIT = 0 once integration of equations has begun.
INITBB	Secondary initialization flag. INITBB is initially 1 and is set to 0 after first calls of ADVINT and CHMINT.
IPRESS	Bypass control variable for pressure (see Section 3).
ISSETL	Bypass control variable for settling velocity (see Section 3).
ISHEAR	Bypass control variable for horizontal wind shear (see Section 3).
ISLDER	Parameter passed to subroutine ADVINT. Acts as a bypass variable for subroutine DERIV. DERIV is bypassed when IDIFF, IVERT, ITEMP, and IPRESS are all zero.
ISSAT (I)	Flag specifying whether advection-diffusion component of energy-balance equation is being treated as unsaturated (ISSAT = 0) or saturated (ISSAT = 1) during current major computation loop.

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
ITCOLL	Specifies output mode to mass storage: zero → no output, negative → unaveraged output every DTCOLL secs, positive → averaged output every DTCOLL secs.
ITEMP	Bypass control variable for temperature (energy balance equation) (See Section 3).
ITOP (K)	Top boundary condition designator for computed species: positive → flux specified, zero or negative → concentration specified.
IVERT	Bypass control variable for vertical air velocity (see Section 3).
JPASSO	Parameter passed to subroutine GEN. When GEN is called from ODEINT, JPASSO = 1 during the predictor pass and JPASSO = 2,3,..., on succes- sive corrector passes. When GEN is called from PLUVIUS (before printed output). JPASSO = 1.
K	Index variable used to specify species number.
KTEMP	Species location variable for temperature. Always required.
KVAPCL	Species location variable for water-vapor + cloud water variable. Required when IFOG = 1 (see Section 3).
L	Index variable used to specify "diffusion regime."
LDIF (K)	Diffusion regime of each species.
LTD	Total number of "diffusion regimes" for a run.
LUNCOL	Parameter specifying logical unit number for output to mass storage (from subroutine COLLECT).
LUNIN	Parameter specifying logical unit number for input.
LUNOUT	Parameter specifying logical unit number for printed output (from subroutine PRINT).

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
MAXITA	Affects filtering. See discussion at end of Appendix A and comments in listing of subroutine FILTER.
MAXITB	Affects filtering. See discussion at end of Appendix A and comments in listing of subroutine FILTER.
MTITLE	Run title which appears on model output (up to 80 characters).
N	Number of vertical grid points.
NAMES (J1,K)	Species name which appears on model output (up to 10 characters).
NCMAX	Parameter for dimensioning arrays. Specifies maximum number of <u>computed</u> species.
NCNSTR	Number of "constrained species", which are computed by methods that do not involve the mass- or energy-balance equations.
NCOMP	Number of "computed species", which are modeled via the finite-difference approximations to the mass-balance or energy-balance equations.
NCORR	Number of corrector passes used in subroutine ODEINT (see Appendix B).
NCTMAX	Parameter for dimensioning arrays. Specifies maximum number of <u>computed</u> and <u>constrained</u> species.
NFILTR	Specifies how often filtering is applied to solution to advection-diffusion component. Filtering occurs every NFILTR steps. (Suggested value=1)
NFSET	Affects filtering. See discussion at end of Appendix A and comments in listing of subroutine FILTER.
NFSRCH	Affects filtering. See discussion at end of Appendix A and comments in listing of subroutine FILTER.

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
NM1	N-1.
NNAMMX	Parameter for dimensioning NAMES array NNAMMX = NCTMAX+2.
NPRINT	Specifies frequency of printed output when output is desired after a fixed number of major computation loops.
NTOT	Total number of species, NCOMP+NCNSTR.
NZMAX	Parameter for dimensioning arrays. Specifies maximum number of vertical grid points.
PRESS (I)	Air pressure. [dyne/cm ²]
PRESSØ	Pressure at bottom of grid at start of computation. [dyne/cm ²]
RATESF (K)	Values of pseudo first-order decay coefficient above which a species is considered to have stiff behavior (see Appendix B).
TCLOCK	Current model time. Because of the splitting of the advection-diffusion and generation components of the equations, model time is somewhat ill-defined during a major computation step. TCLOCK holds the model time at the start and end of each major integration step, at the start of each advection-diffusion integration step, and at the start of each generation integration step. During the integration of the generation component, model time varies from TCLOCK to TCLOCK+2·DT as the integration progresses, and is held by the variables TS and TN in subroutine ODEINT and TGEN in subroutine GEN. [sec]
TEMPØ	Temperature of bottom of grid at start of computation. [K]
TGEN	Parameter passed to subroutine GEN specifying current model time. [sec]
TNEXT	Model time at end of current advection-diffusion integration step. [sec]

TABLE C-19 Continued

<u>Variable</u>	<u>Description</u>
TPRINT	Holds the time at which printed output will next occur, when output is requested at fixed time intervals. [sec]
TSTART	Model time at beginning of computation. [sec]
TSTOP	Model time at which computation terminates. [sec]
TSTRTO	Parameter passed to subroutine ODEINT, specifying the model time at the start of the integration time interval. [sec]
URATIO (I)	u^*/u_A of Eq. (13).
UVEC (J1,I)	XV in Eq. (A12).
WAGRID (I)	Grid vertical velocity. w_{Ao} in Eq. (8) or $w_{Ao} (u_A/u_{Ao})$ in Eq. (11). [cm/sec]
WAP (I)	Component of vertical <u>air</u> velocity relative to grid. w_A' in Eq. (8) or w_A'' in Eq. (11). [cm/sec]
WR (I,K)	Settling velocity. [cm/sec, signed negative]
WVAR (I)	Working array, holds $WR(I,K)+WAP(I)$ for species currently being treated in subroutine ADVINT. [cm/sec]
Z (I)	Relative height of each grid position. Total height = $Z(I) + GLEVL$. $Z(I)$ is constant in time, while GLEVL can change. [cm]

APPENDIX D

EXAMPLE APPLICATION 2 MODEL OUTPUT LISTINGS

This appendix contains the printed model output for Example Application 2. Table D-1 is the output heading page. Tables D-2 through D-6 contain output at model times of 0, 1, 2, 3, and 4 hours.

TABLE D-1. Output Heading Page From Example Application 2

```

+++++
+
+   PLUVIUS   REACTIVE   STORM   MODEL   (MOD 5.0)   +
+
+++++

```

RUN ID: EXAMPLE RUN 2 - PLUVIUS MOD 5.0 USER MANUAL

COMPUTED SPECIES	TOP B.C.	BOTTOM B.C.	DIFFUS. REGIME	FILTER FACT.
1 TEMP	FLUX	FLUX	1	0.00
2 VAPCL	FLUX	FLUX	2	0.00
3 RAIN	FLUX	OUTFLOW	3	0.10
4 SNOW	FLUX	OUTFLOW	4	0.10
5 SO2-GC	FLUX	FLUX	2	0.00
6 SO2-R	FLUX	OUTFLOW	3	0.10
7 SO2-S	FLUX	OUTFLOW	4	0.10
8 SO4-A	FLUX	FLUX	2	0.00
9 SO4-C	FLUX	FLUX	2	0.00
10 SO4-R	FLUX	OUTFLOW	3	0.10
11 SO4-S	FLUX	OUTFLOW	4	0.10
12 H2O2-GC	FLUX	FLUX	2	0.00
13 H2O2-R	FLUX	OUTFLOW	3	0.10
14 H2O2-S	FLUX	OUTFLOW	4	0.10
15 O3-G	FLUX	FLUX	2	0.00

CONSTRAINED SPECIES

```

16 CLOUD
17 HION-C
18 HION-R
19 SO2-G
20 SO2-C

21 H2O2-G
22 H2O2-C

```

CONTROL DATA

```

IGEN   1          IPRESS  1          IVERT   1
IDIFF  1          ISETTL  1          IFOG    1
ITEMP  1          IBOUND  0          ISHEAR  0

TSTART   0.0  ( 0.00 HRS)          NPRINT      0
TSTOP   14400.0  ( 4.00 HRS)        DTPRIN    3600.0
                                          DTCOLL    180.0

```

UNITS USED IN PLUVIUS ARE CGS:

```

TIME          SEC
HEIGHT        CM
VELOCITY      CM/SEC
TEMPERATURE   DEG K
MASS          GM
PRESSURE      DYNES/CM**2
ENERGY        ERGS
CONCENTRATION GM MOLE/CM**3

```

(NOTE: THIS IS CONCENTRATION PER VOLUME OF TOTAL SPACE (AIR),
NOT CONCENTRATION PER VOLUME OF LIQUID)

ALL OUTPUT IN THESE UNITS UNLESS OTHERWISE NOTED

TABLE D-2. Example Application 2 Model Output at TCLOCK = 0 Hours

TCLOCK DT	0.00 60.00	(0.000 HRS)	GLEVL (KM) 0.000 WAGRID(1) 0.00								
Z (KM)	TEMP	VAPCL	RAIN	SNOW	SO2-GC	SO2-R	SO2-S	SO4-A	SO4-C	SO4-R	SO4-S
5.000	0.2597E+03	0.9064E-07	0.1000E-16	0.1000E-16	0.4973E-13	0.1000E-23	0.1000E-23	0.4973E-14	0.1000E-23	0.1000E-23	0.1000E-23
4.800	0.2611E+03	0.1009E-06	0.1000E-16	0.1000E-16	0.5078E-13	0.1000E-23	0.1000E-23	0.5078E-14	0.1000E-23	0.1000E-23	0.1000E-23
4.600	0.2625E+03	0.1119E-06	0.1000E-16	0.1000E-16	0.5185E-13	0.1000E-23	0.1000E-23	0.5185E-14	0.1000E-23	0.1000E-23	0.1000E-23
4.400	0.2638E+03	0.1237E-06	0.1000E-16	0.1000E-16	0.5295E-13	0.1000E-23	0.1000E-23	0.5295E-14	0.1000E-23	0.1000E-23	0.1000E-23
4.200	0.2651E+03	0.1364E-06	0.1000E-16	0.1000E-16	0.5406E-13	0.1000E-23	0.1000E-23	0.5406E-14	0.1000E-23	0.1000E-23	0.1000E-23
4.000	0.2664E+03	0.1499E-06	0.1000E-16	0.1000E-16	0.5520E-13	0.1000E-23	0.1000E-23	0.5520E-14	0.1000E-23	0.1000E-23	0.1000E-23
3.800	0.2677E+03	0.1643E-06	0.1000E-16	0.1000E-16	0.5637E-13	0.1000E-23	0.1000E-23	0.5637E-14	0.1000E-23	0.1000E-23	0.1000E-23
3.600	0.2689E+03	0.1797E-06	0.1000E-16	0.1000E-16	0.5755E-13	0.1000E-23	0.1000E-23	0.5755E-14	0.1000E-23	0.1000E-23	0.1000E-23
3.400	0.2701E+03	0.1959E-06	0.1000E-16	0.1000E-16	0.5876E-13	0.1000E-23	0.1000E-23	0.5876E-14	0.1000E-23	0.1000E-23	0.1000E-23
3.200	0.2713E+03	0.2132E-06	0.1000E-16	0.1000E-16	0.6000E-13	0.1000E-23	0.1000E-23	0.6000E-14	0.1000E-23	0.1000E-23	0.1000E-23
3.000	0.2725E+03	0.2314E-06	0.1000E-16	0.1000E-16	0.6126E-13	0.1000E-23	0.1000E-23	0.6126E-14	0.1000E-23	0.1000E-23	0.1000E-23
2.800	0.2737E+03	0.2506E-06	0.1000E-16	0.1000E-16	0.6255E-13	0.1000E-23	0.1000E-23	0.6255E-14	0.1000E-23	0.1000E-23	0.1000E-23
2.600	0.2748E+03	0.2709E-06	0.1000E-16	0.1000E-16	0.6386E-13	0.1000E-23	0.1000E-23	0.6386E-14	0.1000E-23	0.1000E-23	0.1000E-23
2.400	0.2759E+03	0.2922E-06	0.1000E-16	0.1000E-16	0.6520E-13	0.1000E-23	0.1000E-23	0.6520E-14	0.1000E-23	0.1000E-23	0.1000E-23
2.200	0.2770E+03	0.3146E-06	0.1000E-16	0.1000E-16	0.6656E-13	0.1000E-23	0.1000E-23	0.6656E-14	0.1000E-23	0.1000E-23	0.1000E-23
2.000	0.2781E+03	0.3382E-06	0.1000E-16	0.1000E-16	0.6796E-13	0.1000E-23	0.1000E-23	0.6796E-14	0.1000E-23	0.1000E-23	0.1000E-23
1.800	0.2792E+03	0.3628E-06	0.1000E-16	0.1000E-16	0.6938E-13	0.1000E-23	0.1000E-23	0.6938E-14	0.1000E-23	0.1000E-23	0.1000E-23
1.600	0.2802E+03	0.3886E-06	0.1000E-16	0.1000E-16	0.7083E-13	0.1000E-23	0.1000E-23	0.7083E-14	0.1000E-23	0.1000E-23	0.1000E-23
1.400	0.2813E+03	0.4157E-06	0.1000E-16	0.1000E-16	0.3615E-12	0.1000E-23	0.1000E-23	0.3615E-13	0.1000E-23	0.1000E-23	0.1000E-23
1.200	0.2823E+03	0.4439E-06	0.1000E-16	0.1000E-16	0.3690E-12	0.1000E-23	0.1000E-23	0.3690E-13	0.1000E-23	0.1000E-23	0.1000E-23
1.000	0.2833E+03	0.4733E-06	0.1000E-16	0.1000E-16	0.3767E-12	0.1000E-23	0.1000E-23	0.3767E-13	0.1000E-23	0.1000E-23	0.1000E-23
0.800	0.2843E+03	0.5041E-06	0.1000E-16	0.1000E-16	0.3845E-12	0.1000E-23	0.1000E-23	0.3845E-13	0.1000E-23	0.1000E-23	0.1000E-23
0.600	0.2853E+03	0.5361E-06	0.1000E-16	0.1000E-16	0.3925E-12	0.1000E-23	0.1000E-23	0.3925E-13	0.1000E-23	0.1000E-23	0.1000E-23
0.400	0.2862E+03	0.5694E-06	0.1000E-16	0.1000E-16	0.4007E-12	0.1000E-23	0.1000E-23	0.4007E-13	0.1000E-23	0.1000E-23	0.1000E-23
0.200	0.2872E+03	0.6041E-06	0.1000E-16	0.1000E-16	0.4089E-12	0.1000E-23	0.1000E-23	0.4089E-13	0.1000E-23	0.1000E-23	0.1000E-23
0.000	0.2881E+03	0.6402E-06	0.1000E-16	0.1000E-16	0.4174E-12	0.1000E-23	0.1000E-23	0.4174E-13	0.1000E-23	0.1000E-23	0.1000E-23

TABLE D-2 Continued

TCLOCK DT	0.00 60.00	(0.000 HRS)			GLEVL (KM) WAGRID(1)	0.000 0.00						
Z (KM)	H2O2-GC	H2O2-R	H2O2-S	O3-G	CLOUD	HION-C	HION-R	SO2-G	SO2-C	H2O2-G	H2O2-C	
5.000	0.4973E-14	0.1000E-23	0.1000E-23	0.1243E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4973E-13	0.0000E+00	0.4973E-14	0.0000E+00	
4.800	0.5078E-14	0.1000E-23	0.1000E-23	0.1269E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5078E-13	0.0000E+00	0.5078E-14	0.0000E+00	
4.600	0.5185E-14	0.1000E-23	0.1000E-23	0.1296E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5185E-13	0.0000E+00	0.5185E-14	0.0000E+00	
4.400	0.5295E-14	0.1000E-23	0.1000E-23	0.1324E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5295E-13	0.0000E+00	0.5295E-14	0.0000E+00	
4.200	0.5406E-14	0.1000E-23	0.1000E-23	0.1352E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5406E-13	0.0000E+00	0.5406E-14	0.0000E+00	
4.000	0.5520E-14	0.1000E-23	0.1000E-23	0.1380E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5520E-13	0.0000E+00	0.5520E-14	0.0000E+00	
3.800	0.5637E-14	0.1000E-23	0.1000E-23	0.1409E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5637E-13	0.0000E+00	0.5637E-14	0.0000E+00	
3.600	0.5755E-14	0.1000E-23	0.1000E-23	0.1439E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5755E-13	0.0000E+00	0.5755E-14	0.0000E+00	
3.400	0.5876E-14	0.1000E-23	0.1000E-23	0.1469E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.5876E-13	0.0000E+00	0.5876E-14	0.0000E+00	
3.200	0.6000E-14	0.1000E-23	0.1000E-23	0.1500E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6000E-13	0.0000E+00	0.6000E-14	0.0000E+00	
3.000	0.6126E-14	0.1000E-23	0.1000E-23	0.1532E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6126E-13	0.0000E+00	0.6126E-14	0.0000E+00	
2.800	0.6255E-14	0.1000E-23	0.1000E-23	0.1564E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6255E-13	0.0000E+00	0.6255E-14	0.0000E+00	
2.600	0.6386E-14	0.1000E-23	0.1000E-23	0.1596E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6386E-13	0.0000E+00	0.6386E-14	0.0000E+00	
2.400	0.6520E-14	0.1000E-23	0.1000E-23	0.1630E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6520E-13	0.0000E+00	0.6520E-14	0.0000E+00	
2.200	0.6656E-14	0.1000E-23	0.1000E-23	0.1664E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6656E-13	0.0000E+00	0.6656E-14	0.0000E+00	
2.000	0.6796E-14	0.1000E-23	0.1000E-23	0.1699E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6796E-13	0.0000E+00	0.6796E-14	0.0000E+00	
1.800	0.6938E-14	0.1000E-23	0.1000E-23	0.1734E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.6938E-13	0.0000E+00	0.6938E-14	0.0000E+00	
1.600	0.7083E-14	0.1000E-23	0.1000E-23	0.1771E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.7083E-13	0.0000E+00	0.7083E-14	0.0000E+00	
1.400	0.3615E-13	0.1000E-23	0.1000E-23	0.1808E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.3615E-12	0.0000E+00	0.3615E-13	0.0000E+00	
1.200	0.3690E-13	0.1000E-23	0.1000E-23	0.1845E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.3690E-12	0.0000E+00	0.3690E-13	0.0000E+00	
1.000	0.3767E-13	0.1000E-23	0.1000E-23	0.1884E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.3767E-12	0.0000E+00	0.3767E-13	0.0000E+00	
0.800	0.3845E-13	0.1000E-23	0.1000E-23	0.1923E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.3845E-12	0.0000E+00	0.3845E-13	0.0000E+00	
0.600	0.3925E-13	0.1000E-23	0.1000E-23	0.1963E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.3925E-12	0.0000E+00	0.3925E-13	0.0000E+00	
0.400	0.4007E-13	0.1000E-23	0.1000E-23	0.2003E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4007E-12	0.0000E+00	0.4007E-13	0.0000E+00	
0.200	0.4089E-13	0.1000E-23	0.1000E-23	0.2045E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4089E-12	0.0000E+00	0.4089E-13	0.0000E+00	
0.000	0.4174E-13	0.1000E-23	0.1000E-23	0.2087E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4174E-12	0.0000E+00	0.4174E-13	0.0000E+00	

TABLE D-2 Continued

TCLOCK	0.00	(	0.000 HRS)	GLEVL (KM)	0.000
DT	60.00			WAGRID(1)	0.00
Z (KM)	P		CS		
5.000	0.5369E+06		0.2486E-04		
4.800	0.5512E+06		0.2539E-04		
4.600	0.5658E+06		0.2593E-04		
4.400	0.5806E+06		0.2647E-04		
4.200	0.5958E+06		0.2703E-04		
4.000	0.6114E+06		0.2760E-04		
3.800	0.6272E+06		0.2818E-04		
3.600	0.6434E+06		0.2878E-04		
3.400	0.6599E+06		0.2938E-04		
3.200	0.6768E+06		0.3000E-04		
3.000	0.6940E+06		0.3063E-04		
2.800	0.7116E+06		0.3127E-04		
2.600	0.7295E+06		0.3193E-04		
2.400	0.7478E+06		0.3260E-04		
2.200	0.7666E+06		0.3328E-04		
2.000	0.7857E+06		0.3398E-04		
1.800	0.8052E+06		0.3469E-04		
1.600	0.8251E+06		0.3541E-04		
1.400	0.8454E+06		0.3615E-04		
1.200	0.8661E+06		0.3690E-04		
1.000	0.8873E+06		0.3767E-04		
0.800	0.9089E+06		0.3845E-04		
0.600	0.9310E+06		0.3925E-04		
0.400	0.9535E+06		0.4007E-04		
0.200	0.9765E+06		0.4089E-04		
0.000	0.1000E+07		0.4174E-04		

TABLE D-3. Example Application 2 Model Output at TCLOCK = 1 Hours

TCLOCK	3667.88	(1.019 HRS)	GLEVL (KM) 0.864									
DT	35.12		WAGRID(1) 14.98									
Z(KM)	TEMP	VAPCL	RAIN	SNOW	SO2-GC	SO2-R	SO2-S	SO4-A	SO4-C	SO4-R	SO4-S	
5.864	0.2528E+03	0.8909E-07	0.6524E-12	0.3290E-09	0.3991E-13	0.9482E-19	0.6448E-18	0.3618E-15	0.9713E-14	0.1990E-18	0.2578E-17	
5.664	0.2544E+03	0.9304E-07	0.1867E-11	0.7141E-09	0.4100E-13	0.1288E-18	0.2410E-17	0.2052E-15	0.9771E-14	0.6940E-18	0.1276E-16	
5.464	0.2558E+03	0.1012E-06	0.2063E-11	0.1259E-08	0.4195E-13	0.1462E-18	0.5519E-17	0.5795E-16	0.9993E-14	0.7978E-18	0.3460E-16	
5.264	0.2572E+03	0.1116E-06	0.2206E-11	0.1743E-08	0.4284E-13	0.1483E-18	0.9614E-17	0.1049E-16	0.1023E-13	0.8386E-18	0.6477E-16	
5.064	0.2586E+03	0.1235E-06	0.2480E-11	0.2149E-08	0.4371E-13	0.1608E-18	0.1441E-16	0.1426E-17	0.1049E-13	0.9064E-18	0.1005E-15	
4.864	0.2600E+03	0.1364E-06	0.3121E-11	0.2086E-08	0.4461E-13	0.1852E-18	0.1478E-16	0.5976E-18	0.1077E-13	0.1084E-17	0.1024E-15	
4.664	0.2613E+03	0.1501E-06	0.3797E-11	0.1254E-08	0.4554E-13	0.2168E-18	0.7872E-17	0.3285E-17	0.1106E-13	0.1264E-17	0.5330E-16	
4.464	0.2627E+03	0.1644E-06	0.5474E-11	0.4276E-09	0.4648E-13	0.3056E-18	0.1751E-17	0.1588E-16	0.1131E-13	0.1728E-17	0.1133E-16	
4.264	0.2639E+03	0.1793E-06	0.7512E-11	0.1194E-09	0.4743E-13	0.3977E-18	0.1853E-18	0.4067E-16	0.1154E-13	0.2338E-17	0.1116E-17	
4.064	0.2652E+03	0.1951E-06	0.1077E-10	0.4125E-10	0.4840E-13	0.5561E-18	0.3064E-19	0.1594E-16	0.1185E-13	0.3146E-17	0.2022E-18	
3.864	0.2664E+03	0.2119E-06	0.1351E-10	0.1144E-10	0.4942E-13	0.6557E-18	0.2767E-20	0.3301E-17	0.1213E-13	0.3989E-17	0.1372E-19	
3.664	0.2676E+03	0.2295E-06	0.2158E-10	0.2825E-11	0.5046E-13	0.1023E-17	0.7049E-21	0.4623E-18	0.1239E-13	0.5992E-17	0.5236E-20	
3.464	0.2688E+03	0.2480E-06	0.2975E-10	0.5097E-12	0.5156E-13	0.1323E-17	0.1299E-21	0.5031E-19	0.1265E-13	0.8436E-17	0.5087E-21	
3.264	0.2700E+03	0.2675E-06	0.3941E-10	0.7005E-13	0.5287E-13	0.1688E-17	0.4697E-22	0.2531E-19	0.1296E-13	0.1079E-16	0.3552E-21	
3.064	0.2712E+03	0.2880E-06	0.6321E-10	0.1102E-13	0.5525E-13	0.2637E-17	0.1365E-22	0.2586E-18	0.1350E-13	0.1758E-16	0.7557E-22	
2.864	0.2723E+03	0.3094E-06	0.7912E-10	0.2223E-14	0.6219E-13	0.3262E-17	0.5569E-23	0.2534E-17	0.1505E-13	0.2189E-16	0.2842E-22	
2.664	0.2735E+03	0.3319E-06	0.1283E-09	0.5059E-15	0.8387E-13	0.5738E-17	0.2264E-23	0.1874E-16	0.1985E-13	0.4435E-16	0.9242E-23	
2.464	0.2746E+03	0.3555E-06	0.1567E-09	0.8458E-16	0.1364E-12	0.8564E-17	0.1125E-23	0.9365E-16	0.3134E-13	0.6273E-16	0.1985E-23	
2.264	0.2756E+03	0.3800E-06	0.2338E-09	0.1066E-16	0.2154E-12	0.1474E-16	0.1000E-23	0.2458E-15	0.4858E-13	0.1450E-15	0.1003E-23	
2.064	0.2767E+03	0.4058E-06	0.2742E-09	0.1000E-16	0.2714E-12	0.1716E-16	0.1000E-23	0.1072E-15	0.6111E-13	0.2226E-15	0.1000E-23	
1.864	0.2777E+03	0.4327E-06	0.3856E-09	0.1000E-16	0.2993E-12	0.2291E-16	0.1000E-23	0.7527E-16	0.6718E-13	0.3640E-15	0.1000E-23	
1.664	0.2787E+03	0.4604E-06	0.5213E-09	0.1000E-16	0.3126E-12	0.2874E-16	0.1000E-23	0.2763E-15	0.6975E-13	0.5390E-15	0.1000E-23	
1.464	0.2798E+03	0.4884E-06	0.6419E-09	0.1000E-16	0.3211E-12	0.3391E-16	0.1000E-23	0.9388E-15	0.7052E-13	0.6712E-15	0.1000E-23	
1.264	0.2808E+03	0.5155E-06	0.8152E-09	0.1000E-16	0.3285E-12	0.4127E-16	0.1000E-23	0.2108E-14	0.7023E-13	0.8724E-15	0.1000E-23	
1.064	0.2818E+03	0.5386E-06	0.1184E-08	0.1000E-16	0.3362E-12	0.5726E-16	0.1000E-23	0.3310E-14	0.6934E-13	0.1268E-14	0.1000E-23	
0.864	0.2828E+03	0.5545E-06	0.1551E-08	0.1000E-16	0.3438E-12	0.6905E-16	0.1000E-23	0.2623E-14	0.7021E-13	0.1784E-14	0.1000E-23	

TABLE D-3 Continued

TCLOCK	3667.88	(1.019 HRS)		GLEVL (KM) 0.864							
DT	35.12			WAGRID(1) 14.98							
Z (KM)	H2O2-GC	H2O2-R	H2O2-S	O3-G	CLOUD	HION-C	HION-R	SO2-G	SO2-C	H2O2-G	H2O2-C
5.864	0.9946E-18	0.1498E-22	0.4916E-19	0.1135E-11	0.3102E-07	0.2595E-13	0.5359E-18	0.3707E-13	0.2839E-14	0.1859E-19	0.9760E-18
5.664	0.1601E-17	0.9661E-22	0.9032E-19	0.1159E-11	0.2731E-07	0.2512E-13	0.1766E-17	0.3882E-13	0.2177E-14	0.3943E-19	0.1561E-17
5.464	0.2828E-17	0.1884E-21	0.1945E-18	0.1183E-11	0.2727E-07	0.2553E-13	0.2009E-17	0.3996E-13	0.1993E-14	0.8042E-19	0.2747E-17
5.264	0.4269E-17	0.3009E-21	0.4389E-18	0.1208E-11	0.2884E-07	0.2637E-13	0.2121E-17	0.4085E-13	0.1991E-14	0.1321E-18	0.4137E-17
5.064	0.6006E-17	0.4419E-21	0.8605E-18	0.1234E-11	0.3105E-07	0.2741E-13	0.2317E-17	0.4167E-13	0.2048E-14	0.1979E-18	0.5809E-17
4.864	0.8208E-17	0.7276E-21	0.1014E-17	0.1260E-11	0.3354E-07	0.2857E-13	0.2811E-17	0.4249E-13	0.2120E-14	0.2856E-18	0.7922E-17
4.664	0.1099E-16	0.1086E-20	0.5714E-18	0.1286E-11	0.3602E-07	0.2972E-13	0.3317E-17	0.4336E-13	0.2182E-14	0.4049E-18	0.1059E-16
4.464	0.1438E-16	0.1970E-20	0.1133E-18	0.1313E-11	0.3829E-07	0.3077E-13	0.4606E-17	0.4426E-13	0.2219E-14	0.5640E-18	0.1382E-16
4.264	0.1814E-16	0.3093E-20	0.8272E-20	0.1340E-11	0.4048E-07	0.3176E-13	0.6259E-17	0.4518E-13	0.2247E-14	0.7576E-18	0.1738E-16
4.064	0.2174E-16	0.5355E-20	0.2897E-20	0.1369E-11	0.4297E-07	0.3295E-13	0.8589E-17	0.4611E-13	0.2290E-14	0.9584E-18	0.2079E-16
3.864	0.2672E-16	0.7070E-20	0.1931E-21	0.1398E-11	0.4522E-07	0.3404E-13	0.1085E-16	0.4711E-13	0.2309E-14	0.1252E-17	0.2547E-16
3.664	0.3298E-16	0.1412E-19	0.9384E-22	0.1427E-11	0.4727E-07	0.3505E-13	0.1663E-16	0.4815E-13	0.2311E-14	0.1649E-17	0.3133E-16
3.464	0.4032E-16	0.2104E-19	0.7598E-23	0.1458E-11	0.4929E-07	0.3605E-13	0.2325E-16	0.4925E-13	0.2309E-14	0.2151E-17	0.3817E-16
3.264	0.4820E-16	0.3270E-19	0.4661E-23	0.1488E-11	0.5128E-07	0.3712E-13	0.3008E-16	0.5057E-13	0.2308E-14	0.2746E-17	0.4553E-16
3.064	0.5382E-16	0.5888E-19	0.1580E-23	0.1520E-11	0.5325E-07	0.3863E-13	0.4876E-16	0.5293E-13	0.2324E-14	0.3260E-17	0.5056E-16
2.864	0.4669E-16	0.7362E-19	0.1201E-23	0.1551E-11	0.5519E-07	0.4202E-13	0.6081E-16	0.5978E-13	0.2413E-14	0.3009E-17	0.4369E-16
2.664	0.1975E-16	0.7468E-19	0.1062E-23	0.1584E-11	0.5710E-07	0.5145E-13	0.1151E-15	0.8119E-13	0.2680E-14	0.1353E-17	0.1840E-16
2.464	0.2235E-17	0.4070E-19	0.1007E-23	0.1617E-11	0.5907E-07	0.7337E-13	0.1566E-15	0.1333E-12	0.3109E-14	0.1622E-18	0.2073E-17
2.264	0.1006E-18	0.1123E-19	0.1000E-23	0.1650E-11	0.6126E-07	0.1061E-12	0.3295E-15	0.2119E-12	0.3476E-14	0.7691E-20	0.9288E-19
2.064	0.3259E-20	0.2026E-20	0.1000E-23	0.1685E-11	0.6439E-07	0.1302E-12	0.4843E-15	0.2677E-12	0.3723E-14	0.2581E-21	0.3001E-20
1.864	0.1026E-21	0.3043E-21	0.1000E-23	0.1721E-11	0.6677E-07	0.1421E-12	0.7761E-15	0.2955E-12	0.3802E-14	0.8527E-23	0.9407E-22
1.664	0.4424E-23	0.5033E-22	0.1000E-23	0.1757E-11	0.6851E-07	0.1473E-12	0.1137E-14	0.3088E-12	0.3788E-14	0.3892E-24	0.4034E-23
1.464	0.1040E-23	0.9417E-23	0.1000E-23	0.1794E-11	0.6931E-07	0.1490E-12	0.1414E-14	0.3174E-12	0.3704E-14	0.9786E-25	0.9417E-24
1.264	0.1310E-23	0.2885E-23	0.1000E-23	0.1833E-11	0.6787E-07	0.1481E-12	0.1832E-14	0.3251E-12	0.3446E-14	0.1356E-24	0.1174E-23
1.064	0.3302E-23	0.2028E-23	0.1000E-23	0.1874E-11	0.6032E-07	0.1445E-12	0.2664E-14	0.3335E-12	0.2703E-14	0.4092E-24	0.2893E-23
0.864	0.5700E-23	0.1987E-23	0.1000E-23	0.1914E-11	0.4395E-07	0.1420E-12	0.3718E-14	0.3424E-12	0.1426E-14	0.9938E-24	0.4706E-23

TABLE D-3 Continued

TCLOCK	3667.88	(1.019 HRS)	GLEVL (KM)	0.864
DT	35.12		WAGRID(1)	14.98
Z (KM)	P	CS		
5.864	0.4775E+06	0.2271E-04		
5.664	0.4905E+06	0.2319E-04		
5.464	0.5038E+06	0.2369E-04		
5.264	0.5174E+06	0.2419E-04		
5.064	0.5313E+06	0.2471E-04		
4.864	0.5455E+06	0.2523E-04		
4.664	0.5600E+06	0.2577E-04		
4.464	0.5748E+06	0.2632E-04		
4.264	0.5899E+06	0.2688E-04		
4.064	0.6053E+06	0.2745E-04		
3.864	0.6211E+06	0.2804E-04		
3.664	0.6372E+06	0.2863E-04		
3.464	0.6536E+06	0.2924E-04		
3.264	0.6704E+06	0.2986E-04		
3.064	0.6875E+06	0.3049E-04		
2.864	0.7050E+06	0.3114E-04		
2.664	0.7229E+06	0.3179E-04		
2.464	0.7412E+06	0.3247E-04		
2.264	0.7598E+06	0.3315E-04		
2.064	0.7788E+06	0.3386E-04		
1.864	0.7983E+06	0.3457E-04		
1.664	0.8181E+06	0.3530E-04		
1.464	0.8384E+06	0.3604E-04		
1.264	0.8591E+06	0.3680E-04		
1.064	0.8802E+06	0.3757E-04		
0.864	0.9017E+06	0.3835E-04		

TABLE D-4. Example Application 2 Model Output at TCLOCK = 2 Hours

TCLOCK	7225.84	(2.007 HRS)	GLEVL (KM)	0.994							
DT	23.53		WAGRID(1)	0.00							
Z (KM)	TEMP	VAPCL	RAIN	SNOW	SO2-GC	SO2-R	SO2-S	SO4-A	SO4-C	SO4-R	SO4-S
5.994	0.2518E+03	0.8468E-07	0.2748E-11	0.5527E-09	0.3554E-13	0.6007E-18	0.1276E-17	0.2005E-15	0.1313E-13	0.4033E-17	0.2329E-16
5.794	0.2534E+03	0.8601E-07	0.2202E-10	0.1190E-08	0.3686E-13	0.1233E-17	0.7355E-17	0.1707E-15	0.1263E-13	0.9627E-17	0.5139E-16
5.594	0.2549E+03	0.9040E-07	0.3217E-10	0.1977E-08	0.3816E-13	0.2319E-17	0.1051E-16	0.9663E-16	0.1203E-13	0.1662E-16	0.8819E-16
5.394	0.2563E+03	0.9725E-07	0.5911E-10	0.3041E-08	0.3914E-13	0.2833E-17	0.2148E-16	0.4052E-16	0.1158E-13	0.3092E-16	0.1662E-15
5.194	0.2578E+03	0.1064E-06	0.8038E-10	0.3413E-08	0.3990E-13	0.4416E-17	0.2678E-16	0.1397E-16	0.1133E-13	0.3958E-16	0.2463E-15
4.994	0.2591E+03	0.1168E-06	0.1291E-09	0.5126E-08	0.4054E-13	0.5535E-17	0.4502E-16	0.5957E-17	0.1111E-13	0.6957E-16	0.4279E-15
4.794	0.2605E+03	0.1287E-06	0.1641E-09	0.5858E-08	0.4114E-13	0.7448E-17	0.5975E-16	0.6930E-17	0.1098E-13	0.7727E-16	0.5524E-15
4.594	0.2618E+03	0.1410E-06	0.2441E-09	0.7257E-08	0.4171E-13	0.9547E-17	0.8093E-16	0.1137E-16	0.1072E-13	0.1271E-15	0.7294E-15
4.394	0.2631E+03	0.1544E-06	0.3050E-09	0.8638E-08	0.4230E-13	0.1190E-16	0.1192E-15	0.1389E-16	0.1050E-13	0.1441E-15	0.1080E-14
4.194	0.2644E+03	0.1680E-06	0.4204E-09	0.9852E-08	0.4289E-13	0.1534E-16	0.1352E-15	0.1023E-16	0.1012E-13	0.1976E-15	0.1210E-14
3.994	0.2656E+03	0.1826E-06	0.5507E-09	0.1144E-07	0.4359E-13	0.1949E-16	0.1969E-15	0.5125E-17	0.9789E-14	0.2427E-15	0.1696E-14
3.794	0.2669E+03	0.1975E-06	0.7322E-09	0.1300E-07	0.4439E-13	0.2557E-16	0.2320E-15	0.1886E-17	0.9265E-14	0.3010E-15	0.1893E-14
3.594	0.2681E+03	0.2132E-06	0.8952E-09	0.1547E-07	0.4560E-13	0.3091E-16	0.3297E-15	0.6529E-18	0.8804E-14	0.3490E-15	0.2622E-14
3.394	0.2693E+03	0.2297E-06	0.1111E-08	0.1710E-07	0.4795E-13	0.3827E-16	0.4220E-15	0.6647E-18	0.8421E-14	0.4174E-15	0.3182E-14
3.194	0.2704E+03	0.2473E-06	0.1340E-08	0.1800E-07	0.5350E-13	0.4814E-16	0.4705E-15	0.2101E-17	0.8476E-14	0.4881E-15	0.3452E-14
2.994	0.2716E+03	0.2655E-06	0.1649E-08	0.1780E-07	0.6654E-13	0.6680E-16	0.4847E-15	0.6560E-17	0.9113E-14	0.6072E-15	0.3479E-14
2.794	0.2727E+03	0.2851E-06	0.2133E-08	0.1410E-07	0.9243E-13	0.1135E-15	0.3972E-15	0.1659E-16	0.1092E-13	0.7101E-15	0.2790E-14
2.594	0.2737E+03	0.3020E-06	0.4947E-08	0.5331E-08	0.1329E-12	0.3409E-15	0.1511E-15	0.2805E-16	0.1200E-13	0.1393E-14	0.1042E-14
2.394	0.2748E+03	0.3197E-06	0.6940E-08	0.1218E-08	0.1843E-12	0.5497E-15	0.3432E-16	0.3257E-16	0.1209E-13	0.2091E-14	0.2348E-15
2.194	0.2759E+03	0.3385E-06	0.7641E-08	0.1857E-09	0.2315E-12	0.7349E-15	0.5203E-17	0.2868E-16	0.1088E-13	0.2587E-14	0.3527E-16
1.994	0.2770E+03	0.3589E-06	0.8064E-08	0.1288E-11	0.2661E-12	0.8837E-15	0.3852E-19	0.3043E-16	0.8812E-14	0.3017E-14	0.2579E-18
1.794	0.2780E+03	0.3812E-06	0.8261E-08	0.1000E-16	0.2887E-12	0.9027E-15	0.1000E-23	0.4571E-16	0.6531E-14	0.3205E-14	0.1000E-23
1.594	0.2791E+03	0.4052E-06	0.8275E-08	0.1000E-16	0.3040E-12	0.8652E-15	0.1000E-23	0.1034E-15	0.4510E-14	0.3372E-14	0.1000E-23
1.394	0.2801E+03	0.4309E-06	0.8285E-08	0.1000E-16	0.3160E-12	0.8203E-15	0.1000E-23	0.4260E-15	0.3044E-14	0.3604E-14	0.1000E-23
1.194	0.2811E+03	0.4568E-06	0.8329E-08	0.1000E-16	0.3270E-12	0.7993E-15	0.1000E-23	0.4340E-14	0.1000E-23	0.3740E-14	0.1000E-23
0.994	0.2823E+03	0.4762E-06	0.8379E-08	0.1000E-16	0.3357E-12	0.7772E-15	0.1000E-23	0.8330E-14	0.1000E-23	0.3809E-14	0.1000E-23

TABLE D-4 Continued

TCLOCK	7225.84	(2.007 HRS)		GLEVL (KM) 0.994		WAGRID(1) 0.00					
DT	23.53										
Z (KM)	H2O2-GC	H2O2-R	H2O2-S	O3-G	CLOUD	HION-C	HION-R	SO2-G	SO2-C	H2O2-G	H2O2-C
5.994	0.1000E-23	0.1000E-23	0.7985E-22	0.1115E-11	0.3125E-07	0.3238E-13	0.8213E-17	0.3322E-13	0.2318E-14	0.1677E-25	0.9832E-24
5.794	0.1000E-23	0.1000E-23	0.1745E-21	0.1140E-11	0.2528E-07	0.2994E-13	0.2351E-16	0.3528E-13	0.1583E-14	0.2412E-25	0.9759E-24
5.594	0.1003E-23	0.1000E-23	0.2997E-21	0.1164E-11	0.2180E-07	0.2794E-13	0.3912E-16	0.3696E-13	0.1194E-14	0.3240E-25	0.9704E-24
5.394	0.1486E-23	0.1000E-23	0.6317E-21	0.1189E-11	0.2011E-07	0.2668E-13	0.7260E-16	0.3815E-13	0.9923E-15	0.5976E-25	0.1426E-23
5.194	0.3551E-23	0.1000E-23	0.9413E-21	0.1214E-11	0.1997E-07	0.2616E-13	0.9412E-16	0.3898E-13	0.9205E-15	0.1647E-24	0.3387E-23
4.994	0.8150E-23	0.1000E-23	0.1431E-20	0.1239E-11	0.2046E-07	0.2588E-13	0.1623E-15	0.3964E-13	0.8992E-15	0.4207E-24	0.7729E-23
4.794	0.1769E-22	0.1000E-23	0.2322E-20	0.1265E-11	0.2168E-07	0.2596E-13	0.1855E-15	0.4022E-13	0.9251E-15	0.9803E-24	0.1671E-22
4.594	0.3546E-22	0.1000E-23	0.3355E-20	0.1292E-11	0.2254E-07	0.2568E-13	0.2986E-15	0.4078E-13	0.9329E-15	0.2136E-23	0.3332E-22
4.394	0.6669E-22	0.1051E-23	0.6360E-20	0.1319E-11	0.2366E-07	0.2555E-13	0.3458E-15	0.4135E-13	0.9558E-15	0.4310E-23	0.6238E-22
4.194	0.1171E-21	0.1230E-23	0.9694E-20	0.1346E-11	0.2432E-07	0.2501E-13	0.4747E-15	0.4194E-13	0.9577E-15	0.8245E-23	0.1088E-21
3.994	0.1963E-21	0.1628E-23	0.1832E-19	0.1375E-11	0.2509E-07	0.2459E-13	0.5918E-15	0.4262E-13	0.9665E-15	0.1496E-22	0.1814E-21
3.794	0.3045E-21	0.2711E-23	0.2917E-19	0.1404E-11	0.2511E-07	0.2362E-13	0.7463E-15	0.4345E-13	0.9443E-15	0.2575E-22	0.2788E-21
3.594	0.4210E-21	0.5007E-23	0.7549E-19	0.1433E-11	0.2505E-07	0.2275E-13	0.8770E-15	0.4467E-13	0.9240E-15	0.3950E-22	0.3815E-21
3.394	0.4599E-21	0.8555E-23	0.1369E-18	0.1463E-11	0.2471E-07	0.2195E-13	0.1059E-14	0.4705E-13	0.9061E-15	0.4815E-22	0.4117E-21
3.194	0.3239E-21	0.1155E-22	0.1805E-18	0.1494E-11	0.2458E-07	0.2202E-13	0.1249E-14	0.5258E-13	0.9240E-15	0.3743E-22	0.2865E-21
2.994	0.1053E-21	0.1252E-22	0.2031E-18	0.1525E-11	0.2417E-07	0.2310E-13	0.1549E-14	0.6555E-13	0.9845E-15	0.1351E-22	0.9177E-22
2.794	0.1525E-22	0.1170E-22	0.1716E-18	0.1557E-11	0.2437E-07	0.2652E-13	0.1863E-14	0.9130E-13	0.1131E-14	0.2115E-23	0.1314E-22
2.594	0.1360E-23	0.8914E-23	0.7263E-19	0.1589E-11	0.2304E-07	0.2819E-13	0.3848E-14	0.1316E-12	0.1284E-14	0.2130E-24	0.1147E-23
2.394	0.1002E-23	0.7139E-23	0.1807E-19	0.1622E-11	0.1807E-07	0.2712E-13	0.5653E-14	0.1833E-12	0.1070E-14	0.2078E-24	0.7942E-24
2.194	0.1000E-23	0.5216E-23	0.2996E-20	0.1656E-11	0.1349E-07	0.2368E-13	0.6756E-14	0.2307E-12	0.8060E-15	0.2783E-24	0.7217E-24
1.994	0.1000E-23	0.3724E-23	0.2731E-22	0.1691E-11	0.9901E-08	0.1893E-13	0.7663E-14	0.2655E-12	0.5868E-15	0.3652E-24	0.6348E-24
1.794	0.1000E-23	0.2186E-23	0.1000E-23	0.1727E-11	0.6969E-08	0.1394E-13	0.8064E-14	0.2883E-12	0.4027E-15	0.4719E-24	0.5281E-24
1.594	0.1000E-23	0.2965E-23	0.1000E-23	0.1765E-11	0.4595E-08	0.9569E-14	0.8378E-14	0.3037E-12	0.2527E-15	0.5967E-24	0.4033E-24
1.394	0.1001E-23	0.2386E-23	0.1000E-23	0.1803E-11	0.2646E-08	0.6343E-14	0.8814E-14	0.3159E-12	0.1244E-15	0.7376E-24	0.2635E-24
1.194	0.1134E-23	0.2012E-23	0.1000E-23	0.1842E-11	0.0000E+00	0.1864E-23	0.9078E-14	0.3270E-12	0.0000E+00	0.1134E-23	0.0000E+00
0.994	0.2979E-23	0.1735E-23	0.1000E-23	0.1880E-11	0.0000E+00	0.1864E-23	0.9219E-14	0.3357E-12	0.0000E+00	0.2979E-23	0.0000E+00

TABLE D-4 Continued

TCLOCK 7225.84 (2.007 HRS)
DT 23.53

GLEVL (KM) 0.994
WAGRID(1) 0.00

Z (KM)	P	CS
5.994	0.4691E+06	0.2240E-04
5.794	0.4820E+06	0.2288E-04
5.594	0.4951E+06	0.2336E-04
5.394	0.5085E+06	0.2386E-04
5.194	0.5222E+06	0.2437E-04
4.994	0.5362E+06	0.2489E-04
4.794	0.5505E+06	0.2542E-04
4.594	0.5651E+06	0.2596E-04
4.394	0.5800E+06	0.2651E-04
4.194	0.5952E+06	0.2708E-04
3.994	0.6108E+06	0.2765E-04
3.794	0.6266E+06	0.2824E-04
3.594	0.6429E+06	0.2884E-04
3.394	0.6594E+06	0.2945E-04
3.194	0.6763E+06	0.3008E-04
2.994	0.6936E+06	0.3072E-04
2.794	0.7112E+06	0.3137E-04
2.594	0.7292E+06	0.3205E-04
2.394	0.7476E+06	0.3272E-04
2.194	0.7664E+06	0.3341E-04
1.994	0.7856E+06	0.3411E-04
1.794	0.8052E+06	0.3483E-04
1.594	0.8251E+06	0.3556E-04
1.394	0.8456E+06	0.3631E-04
1.194	0.8664E+06	0.3707E-04
0.994	0.8877E+06	0.3782E-04

TABLE D-5. Example Application 2 Model Output at TCLOCK = 3 Hours

TCLOCK 10859.12 DT 60.00		(3.016 HRS)		GLEVL (KM) 0.125 WAGRID(1) -15.44							
Z(KM)	TEMP	VAPCL	RAIN	SNOW	SO2-GC	SO2-R	SO2-S	SO4-A	SO4-C	SO4-R	SO4-S
5.125	0.2587E+03	0.8558E-07	0.1012E-13	0.2018E-09	0.3812E-13	0.7028E-21	0.2902E-18	0.1451E-13	0.1000E-23	0.3136E-19	0.6618E-17
4.925	0.2606E+03	0.8794E-07	0.5662E-14	0.2781E-09	0.3926E-13	0.1285E-20	0.2997E-18	0.1420E-13	0.1000E-23	0.1014E-19	0.1522E-16
4.725	0.2623E+03	0.9245E-07	0.1064E-14	0.5768E-09	0.4068E-13	0.1412E-20	0.6705E-18	0.1336E-13	0.1000E-23	0.1281E-20	0.3051E-16
4.525	0.2640E+03	0.9949E-07	0.1000E-16	0.8006E-09	0.4195E-13	0.1587E-20	0.1465E-17	0.1253E-13	0.1000E-23	0.3157E-22	0.5377E-16
4.325	0.2655E+03	0.1086E-06	0.3450E-15	0.1086E-08	0.4296E-13	0.2151E-20	0.2548E-17	0.1182E-13	0.1000E-23	0.2935E-22	0.7742E-16
4.125	0.2669E+03	0.1195E-06	0.1000E-16	0.1555E-08	0.4376E-13	0.3228E-20	0.4122E-17	0.1125E-13	0.1000E-23	0.1000E-23	0.1099E-15
3.925	0.2682E+03	0.1316E-06	0.4592E-14	0.1901E-08	0.4443E-13	0.4550E-20	0.5293E-17	0.1072E-13	0.1000E-23	0.3956E-21	0.1322E-15
3.725	0.2695E+03	0.1447E-06	0.1000E-16	0.2205E-08	0.4504E-13	0.5117E-20	0.6639E-17	0.1017E-13	0.1000E-23	0.1000E-23	0.1580E-15
3.525	0.2708E+03	0.1587E-06	0.1683E-13	0.2606E-08	0.4566E-13	0.5395E-20	0.8064E-17	0.9552E-14	0.1000E-23	0.1762E-20	0.1937E-15
3.325	0.2721E+03	0.1734E-06	0.1367E-11	0.3233E-08	0.4632E-13	0.6119E-19	0.1109E-16	0.8897E-14	0.1000E-23	0.1463E-18	0.2719E-15
3.125	0.2733E+03	0.1890E-06	0.3347E-11	0.3657E-08	0.4714E-13	0.2328E-18	0.1357E-16	0.8187E-14	0.1000E-23	0.4341E-18	0.3326E-15
2.925	0.2746E+03	0.2054E-06	0.7098E-10	0.3674E-08	0.4835E-13	0.1841E-17	0.1462E-16	0.7455E-14	0.1000E-23	0.5879E-18	0.3562E-15
2.725	0.2757E+03	0.2232E-06	0.4529E-09	0.2651E-08	0.5054E-13	0.2137E-16	0.1104E-16	0.6847E-14	0.1000E-23	0.3620E-16	0.2674E-15
2.525	0.2768E+03	0.2439E-06	0.1122E-08	0.1076E-08	0.5475E-13	0.5301E-16	0.4595E-17	0.6676E-14	0.1000E-23	0.1364E-15	0.1110E-15
2.325	0.2778E+03	0.2645E-06	0.1420E-08	0.1851E-09	0.6384E-13	0.7122E-16	0.8008E-18	0.6736E-14	0.1000E-23	0.1785E-15	0.1930E-16
2.125	0.2789E+03	0.2854E-06	0.1201E-08	0.1000E-16	0.8056E-13	0.6543E-16	0.1000E-23	0.7038E-14	0.1000E-23	0.1427E-15	0.1000E-23
1.925	0.2799E+03	0.3059E-06	0.9317E-09	0.1000E-16	0.1071E-12	0.5759E-16	0.1000E-23	0.7356E-14	0.1000E-23	0.1144E-15	0.1000E-23
1.725	0.2810E+03	0.3257E-06	0.7589E-09	0.1000E-16	0.1439E-12	0.5578E-16	0.1000E-23	0.7351E-14	0.1000E-23	0.1021E-15	0.1000E-23
1.525	0.2822E+03	0.3477E-06	0.6143E-09	0.1000E-16	0.1887E-12	0.5395E-16	0.1000E-23	0.7285E-14	0.1000E-23	0.8926E-16	0.1000E-23
1.325	0.2835E+03	0.3726E-06	0.4827E-09	0.1000E-16	0.2342E-12	0.4815E-16	0.1000E-23	0.7047E-14	0.1000E-23	0.7604E-16	0.1000E-23
1.125	0.2846E+03	0.3990E-06	0.2885E-09	0.1000E-16	0.2734E-12	0.3482E-16	0.1000E-23	0.6703E-14	0.1000E-23	0.5024E-16	0.1000E-23
0.925	0.2857E+03	0.4265E-06	0.1215E-09	0.1000E-16	0.3038E-12	0.1575E-16	0.1000E-23	0.6504E-14	0.1000E-23	0.2240E-16	0.1000E-23
0.725	0.2868E+03	0.4546E-06	0.3553E-10	0.1000E-16	0.3265E-12	0.4060E-17	0.1000E-23	0.6912E-14	0.1000E-23	0.6798E-17	0.1000E-23
0.525	0.2879E+03	0.4819E-06	0.2946E-11	0.1000E-16	0.3432E-12	0.4738E-18	0.1000E-23	0.8392E-14	0.1000E-23	0.5891E-18	0.1000E-23
0.325	0.2892E+03	0.5052E-06	0.4211E-13	0.1000E-16	0.3551E-12	0.3935E-18	0.1000E-23	0.1066E-13	0.1000E-23	0.9620E-20	0.1000E-23
0.125	0.2909E+03	0.5193E-06	0.1422E-12	0.1000E-16	0.3626E-12	0.2776E-18	0.1000E-23	0.1198E-13	0.1000E-23	0.3089E-19	0.1000E-23

TABLE D-5 Continued

TCLOCK 10859.12 (3.016 HRS)
DT 60.00

GLEVL (KM) 0.125
WAGR1D(1) -15.44

Z (KM)	H2O2-GC	H2O2-R	H2O2-S	O3-G	CLOUD	HION-C	HION-R	SO2-G	SO2-C	H2O2-G	H2O2-C
5.125	0.1309E-23	0.1000E-23	0.1000E-23	0.1219E-11	0.0000E+00	0.1864E-23	0.6102E-19	0.3812E-13	0.0000E+00	0.1309E-23	0.0000E+00
4.925	0.1623E-23	0.1030E-23	0.1000E-23	0.1244E-11	0.0000E+00	0.1864E-23	0.2034E-19	0.3926E-13	0.0000E+00	0.1623E-23	0.0000E+00
4.725	0.2042E-23	0.1057E-23	0.1000E-23	0.1271E-11	0.0000E+00	0.1864E-23	0.2658E-20	0.4068E-13	0.0000E+00	0.2042E-23	0.0000E+00
4.525	0.2592E-23	0.1068E-23	0.1179E-23	0.1299E-11	0.0000E+00	0.1864E-23	0.6138E-22	0.4195E-13	0.0000E+00	0.2592E-23	0.0000E+00
4.325	0.3457E-23	0.1055E-23	0.2115E-23	0.1327E-11	0.0000E+00	0.1864E-23	0.1420E-21	0.4296E-13	0.0000E+00	0.3457E-23	0.0000E+00
4.125	0.4147E-23	0.1033E-23	0.3160E-23	0.1356E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4376E-13	0.0000E+00	0.4147E-23	0.0000E+00
3.925	0.4519E-23	0.1015E-23	0.5894E-23	0.1385E-11	0.0000E+00	0.1864E-23	0.1899E-20	0.4443E-13	0.0000E+00	0.4519E-23	0.0000E+00
3.725	0.4892E-23	0.1011E-23	0.8776E-23	0.1414E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4504E-13	0.0000E+00	0.4892E-23	0.0000E+00
3.525	0.5127E-23	0.1001E-23	0.1587E-22	0.1443E-11	0.0000E+00	0.1864E-23	0.7542E-20	0.4566E-13	0.0000E+00	0.5127E-23	0.0000E+00
3.325	0.4973E-23	0.1000E-23	0.3681E-22	0.1474E-11	0.0000E+00	0.1864E-23	0.6185E-18	0.4632E-13	0.0000E+00	0.4973E-23	0.0000E+00
3.125	0.4978E-23	0.1000E-23	0.6488E-22	0.1504E-11	0.0000E+00	0.1864E-23	0.1656E-17	0.4714E-13	0.0000E+00	0.4978E-23	0.0000E+00
2.925	0.4641E-23	0.1000E-23	0.8804E-22	0.1535E-11	0.0000E+00	0.1864E-23	0.1905E-16	0.4835E-13	0.0000E+00	0.4641E-23	0.0000E+00
2.725	0.3520E-23	0.1000E-23	0.7532E-22	0.1568E-11	0.0000E+00	0.1864E-23	0.1820E-15	0.5054E-13	0.0000E+00	0.3520E-23	0.0000E+00
2.525	0.2582E-23	0.1000E-23	0.3399E-22	0.1601E-11	0.0000E+00	0.1864E-23	0.5381E-15	0.5475E-13	0.0000E+00	0.2582E-23	0.0000E+00
2.325	0.1832E-23	0.1115E-23	0.6961E-23	0.1636E-11	0.0000E+00	0.1864E-23	0.6920E-15	0.6384E-13	0.0000E+00	0.1832E-23	0.0000E+00
2.125	0.1590E-23	0.2636E-23	0.1000E-23	0.1671E-11	0.0000E+00	0.1864E-23	0.5698E-15	0.8056E-13	0.0000E+00	0.1590E-23	0.0000E+00
1.925	0.1562E-23	0.2720E-23	0.1000E-23	0.1705E-11	0.0000E+00	0.1864E-23	0.4489E-15	0.1071E-12	0.0000E+00	0.1562E-23	0.0000E+00
1.725	0.1590E-23	0.2550E-23	0.1000E-23	0.1737E-11	0.0000E+00	0.1864E-23	0.3824E-15	0.1439E-12	0.0000E+00	0.1590E-23	0.0000E+00
1.525	0.1748E-23	0.2285E-23	0.1000E-23	0.1769E-11	0.0000E+00	0.1864E-23	0.3218E-15	0.1887E-12	0.0000E+00	0.1748E-23	0.0000E+00
1.325	0.1976E-23	0.2150E-23	0.1000E-23	0.1806E-11	0.0000E+00	0.1864E-23	0.2639E-15	0.2342E-12	0.0000E+00	0.1976E-23	0.0000E+00
1.125	0.2259E-23	0.2149E-23	0.1000E-23	0.1845E-11	0.0000E+00	0.1864E-23	0.1666E-15	0.2734E-12	0.0000E+00	0.2259E-23	0.0000E+00
0.925	0.2563E-23	0.2209E-23	0.1000E-23	0.1886E-11	0.0000E+00	0.1864E-23	0.7248E-16	0.3038E-12	0.0000E+00	0.2563E-23	0.0000E+00
0.725	0.3006E-23	0.2230E-23	0.1000E-23	0.1926E-11	0.0000E+00	0.1864E-23	0.2166E-16	0.3265E-12	0.0000E+00	0.3006E-23	0.0000E+00
0.525	0.3823E-23	0.2176E-23	0.1000E-23	0.1965E-11	0.0000E+00	0.1864E-23	0.1844E-17	0.3432E-12	0.0000E+00	0.3823E-23	0.0000E+00
0.325	0.5484E-23	0.2229E-23	0.1000E-23	0.2000E-11	0.0000E+00	0.1864E-23	0.2859E-19	0.3551E-12	0.0000E+00	0.5484E-23	0.0000E+00
0.125	0.8821E-23	0.2354E-23	0.1000E-23	0.2032E-11	0.0000E+00	0.1864E-23	0.9356E-19	0.3626E-12	0.0000E+00	0.8821E-23	0.0000E+00

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TABLE D-5 Continued

TCLOCK	10859.12	(3.016 HRS)	GLEVL (KM)	0.125
DT	60.00		WAGRID(1)	-15.44
Z (KM)	P	CS		
5.125	0.5296E+06	0.2462E-04		
4.925	0.5437E+06	0.2510E-04		
4.725	0.5581E+06	0.2559E-04		
4.525	0.5728E+06	0.2610E-04		
4.325	0.5877E+06	0.2663E-04		
4.125	0.6030E+06	0.2718E-04		
3.925	0.6186E+06	0.2774E-04		
3.725	0.6345E+06	0.2831E-04		
3.525	0.6508E+06	0.2890E-04		
3.325	0.6674E+06	0.2950E-04		
3.125	0.6843E+06	0.3011E-04		
2.925	0.7016E+06	0.3073E-04		
2.725	0.7192E+06	0.3137E-04		
2.525	0.7372E+06	0.3204E-04		
2.325	0.7556E+06	0.3271E-04		
2.125	0.7744E+06	0.3340E-04		
1.925	0.7936E+06	0.3410E-04		
1.725	0.8131E+06	0.3480E-04		
1.525	0.8331E+06	0.3550E-04		
1.325	0.8535E+06	0.3621E-04		
1.125	0.8743E+06	0.3694E-04		
0.925	0.8955E+06	0.3769E-04		
0.725	0.9171E+06	0.3846E-04		
0.525	0.9391E+06	0.3923E-04		
0.325	0.9617E+06	0.4000E-04		
0.125	0.9846E+06	0.4071E-04		

TABLE D-6. Example Application 2 Model Output at TCLOCK = 4 Hours

TCLOCK 14459.12 DT 60.00		(4.016 HRS)		GLEVL (KM) -0.013 WAGRID(1) 0.00							
Z (KM)	TEMP	VAPCL	RAIN	SNOW	SO2-GC	SO2-R	SO2-S	SO4-A	SO4-C	SO4-R	SO4-S
4.987	0.2599E+03	0.8844E-07	0.1076E-16	0.1000E-16	0.3908E-13	0.1801E-20	0.1000E-23	0.1398E-13	0.1000E-23	0.1058E-23	0.1000E-23
4.787	0.2618E+03	0.9114E-07	0.1015E-16	0.1000E-16	0.4000E-13	0.2951E-20	0.1000E-23	0.1395E-13	0.1000E-23	0.1011E-23	0.1000E-23
4.587	0.2635E+03	0.9596E-07	0.1044E-16	0.1147E-14	0.4115E-13	0.4390E-20	0.4002E-23	0.1346E-13	0.1000E-23	0.1034E-23	0.7466E-22
4.387	0.2652E+03	0.1029E-06	0.1000E-16	0.4909E-14	0.4232E-13	0.6007E-20	0.1189E-22	0.1279E-13	0.1000E-23	0.1000E-23	0.4227E-21
4.187	0.2667E+03	0.1119E-06	0.1591E-16	0.4330E-12	0.4336E-13	0.7277E-20	0.9909E-21	0.1211E-13	0.1000E-23	0.1457E-23	0.3247E-19
3.987	0.2681E+03	0.1225E-06	0.1000E-16	0.3173E-11	0.4424E-13	0.7920E-20	0.7338E-20	0.1148E-13	0.1000E-23	0.1000E-23	0.2370E-18
3.787	0.2695E+03	0.1344E-06	0.9061E-16	0.1240E-10	0.4499E-13	0.8840E-20	0.2905E-19	0.1089E-13	0.1000E-23	0.7236E-23	0.8949E-18
3.587	0.2708E+03	0.1475E-06	0.1000E-16	0.6171E-10	0.4567E-13	0.9304E-20	0.1472E-18	0.1029E-13	0.1000E-23	0.1000E-23	0.4260E-17
3.387	0.2721E+03	0.1615E-06	0.1182E-14	0.1104E-09	0.4637E-13	0.1249E-19	0.2688E-18	0.9670E-14	0.1000E-23	0.9199E-22	0.7707E-17
3.187	0.2734E+03	0.1766E-06	0.5709E-14	0.1329E-09	0.4717E-13	0.1726E-19	0.3269E-18	0.9023E-14	0.1000E-23	0.4633E-21	0.9340E-17
2.987	0.2746E+03	0.1930E-06	0.1820E-12	0.1351E-09	0.4826E-13	0.3998E-19	0.3350E-18	0.8397E-14	0.1000E-23	0.1420E-19	0.9542E-17
2.787	0.2757E+03	0.2116E-06	0.1591E-11	0.9910E-10	0.5004E-13	0.1342E-18	0.2470E-18	0.7905E-14	0.1000E-23	0.1233E-18	0.7022E-17
2.587	0.2767E+03	0.2328E-06	0.3744E-11	0.3951E-10	0.5336E-13	0.2465E-18	0.9874E-19	0.7671E-14	0.1000E-23	0.2898E-18	0.2804E-17
2.387	0.2778E+03	0.2527E-06	0.2598E-11	0.6400E-11	0.5981E-13	0.1901E-18	0.1602E-19	0.7472E-14	0.1000E-23	0.2012E-18	0.4545E-18
2.187	0.2789E+03	0.2726E-06	0.7007E-12	0.1000E-16	0.7124E-13	0.1036E-18	0.1000E-23	0.7433E-14	0.1000E-23	0.5384E-19	0.1000E-23
1.987	0.2800E+03	0.2926E-06	0.1207E-13	0.1000E-16	0.8966E-13	0.5238E-19	0.1000E-23	0.7524E-14	0.1000E-23	0.1133E-20	0.1000E-23
1.787	0.2812E+03	0.3129E-06	0.2389E-15	0.1000E-16	0.1164E-12	0.2536E-19	0.1000E-23	0.7624E-14	0.1000E-23	0.5348E-22	0.1000E-23
1.587	0.2823E+03	0.3337E-06	0.1000E-16	0.1000E-16	0.1512E-12	0.2333E-19	0.1000E-23	0.7624E-14	0.1000E-23	0.4432E-23	0.1000E-23
1.387	0.2835E+03	0.3559E-06	0.4048E-16	0.1000E-16	0.1912E-12	0.2895E-19	0.1000E-23	0.7505E-14	0.1000E-23	0.2925E-23	0.1000E-23
1.187	0.2847E+03	0.3801E-06	0.1499E-16	0.1000E-16	0.2318E-12	0.3405E-19	0.1000E-23	0.7312E-14	0.1000E-23	0.1797E-23	0.1000E-23
0.987	0.2859E+03	0.4057E-06	0.2087E-16	0.1000E-16	0.2685E-12	0.3811E-19	0.1000E-23	0.7177E-14	0.1000E-23	0.2036E-23	0.1000E-23
0.787	0.2870E+03	0.4322E-06	0.1974E-16	0.1000E-16	0.2990E-12	0.4288E-19	0.1000E-23	0.7314E-14	0.1000E-23	0.1989E-23	0.1000E-23
0.587	0.2882E+03	0.4582E-06	0.2007E-16	0.1000E-16	0.3229E-12	0.5471E-19	0.1000E-23	0.7884E-14	0.1000E-23	0.2003E-23	0.1000E-23
0.387	0.2895E+03	0.4815E-06	0.1997E-16	0.1000E-16	0.3407E-12	0.6721E-19	0.1000E-23	0.8804E-14	0.1000E-23	0.1999E-23	0.1000E-23
0.187	0.2911E+03	0.4999E-06	0.1994E-16	0.1000E-16	0.3532E-12	0.7815E-19	0.1000E-23	0.9693E-14	0.1000E-23	0.1996E-23	0.1000E-23
-0.013	0.2929E+03	0.5117E-06	0.1985E-16	0.1000E-16	0.3613E-12	0.8731E-19	0.1000E-23	0.1014E-13	0.1000E-23	0.1992E-23	0.1000E-23

TABLE D-6 Continued

TCLOCK	14459.12	(4.016 HPS)			GLEVL (KM) -0.013							
DT	60.00				WAGPID(1) 0.00							
Z(KM)	H2O2-GC	H2O2-R	H2O2-S	O3-G	CLOUD	HION-C	HION-R	SO2-G	SO2-C	H2O2-G	H2O2-C	
4.987	0.2611E-21	0.1000E-23	0.1000E-23	0.1237E-11	0.0000E+00	0.1864E-23	0.4695E-23	0.3908E-13	0.0000E+00	0.2611E-21	0.0000E+00	
4.787	0.6995E-21	0.1000E-23	0.1000E-23	0.1262E-11	0.0000E+00	0.1864E-23	0.4452E-23	0.4000E-13	0.0000E+00	0.6995E-21	0.0000E+00	
4.587	0.1126E-20	0.1000E-23	0.1000E-23	0.1288E-11	0.0000E+00	0.1864E-23	0.4568E-23	0.4115E-13	0.0000E+00	0.1126E-20	0.0000E+00	
4.387	0.4653E-21	0.1000E-23	0.1000E-23	0.1316E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4232E-13	0.0000E+00	0.4653E-21	0.0000E+00	
4.187	0.1074E-21	0.1000E-23	0.1000E-23	0.1345E-11	0.0000E+00	0.1864E-23	0.6743E-23	0.4336E-13	0.0000E+00	0.1074E-21	0.0000E+00	
3.987	0.2278E-22	0.1000E-23	0.1000E-23	0.1374E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4424E-13	0.0000E+00	0.2278E-22	0.0000E+00	
3.787	0.8539E-23	0.1000E-23	0.1000E-23	0.1404E-11	0.0000E+00	0.1864E-23	0.3641E-22	0.4499E-13	0.0000E+00	0.8539E-23	0.0000E+00	
3.587	0.7035E-23	0.1000E-23	0.1000E-23	0.1434E-11	0.0000E+00	0.1864E-23	0.4394E-23	0.4567E-13	0.0000E+00	0.7035E-23	0.0000E+00	
3.387	0.7941E-23	0.1000E-23	0.1012E-23	0.1464E-11	0.0000E+00	0.1864E-23	0.4705E-21	0.4637E-13	0.0000E+00	0.7941E-23	0.0000E+00	
3.187	0.1010E-22	0.1000E-23	0.1071E-23	0.1494E-11	0.0000E+00	0.1864E-23	0.2308E-20	0.4717E-13	0.0000E+00	0.1010E-22	0.0000E+00	
2.987	0.9907E-23	0.1000E-23	0.1139E-23	0.1525E-11	0.0000E+00	0.1864E-23	0.7252E-19	0.4826E-13	0.0000E+00	0.9907E-23	0.0000E+00	
2.787	0.9324E-23	0.1000E-23	0.1163E-23	0.1557E-11	0.0000E+00	0.1864E-23	0.6322E-18	0.5004E-13	0.0000E+00	0.9324E-23	0.0000E+00	
2.587	0.6719E-23	0.1046E-23	0.1095E-23	0.1591E-11	0.0000E+00	0.1864E-23	0.1487E-17	0.5336E-13	0.0000E+00	0.6719E-23	0.0000E+00	
2.387	0.7591E-23	0.1352E-23	0.1021E-23	0.1624E-11	0.0000E+00	0.1864E-23	0.1032E-17	0.5981E-13	0.0000E+00	0.7591E-23	0.0000E+00	
2.187	0.1122E-22	0.2909E-23	0.1000E-23	0.1659E-11	0.0000E+00	0.1864E-23	0.2776E-18	0.7124E-13	0.0000E+00	0.1122E-22	0.0000E+00	
1.987	0.1592E-22	0.3399E-23	0.1000E-23	0.1693E-11	0.0000E+00	0.1864E-23	0.5164E-20	0.8966E-13	0.0000E+00	0.1592E-22	0.0000E+00	
1.787	0.2027E-22	0.5867E-23	0.1000E-23	0.1728E-11	0.0000E+00	0.1864E-23	0.1601E-21	0.1164E-12	0.0000E+00	0.2027E-22	0.0000E+00	
1.587	0.1481E-22	0.9216E-23	0.1000E-23	0.1761E-11	0.0000E+00	0.1864E-23	0.1079E-22	0.1512E-12	0.0000E+00	0.1481E-22	0.0000E+00	
1.387	0.1187E-22	0.1326E-22	0.1000E-23	0.1796E-11	0.0000E+00	0.1864E-23	0.1569E-22	0.1912E-12	0.0000E+00	0.1187E-22	0.0000E+00	
1.187	0.1044E-22	0.1662E-22	0.1000E-23	0.1832E-11	0.0000E+00	0.1864E-23	0.7142E-23	0.2318E-12	0.0000E+00	0.1044E-22	0.0000E+00	
0.987	0.9636E-23	0.2019E-22	0.1000E-23	0.1871E-11	0.0000E+00	0.1864E-23	0.9075E-23	0.2685E-12	0.0000E+00	0.9636E-23	0.0000E+00	
0.787	0.9209E-23	0.2286E-22	0.1000E-23	0.1911E-11	0.0000E+00	0.1864E-23	0.8703E-23	0.2990E-12	0.0000E+00	0.9209E-23	0.0000E+00	
0.587	0.9551E-23	0.2501E-22	0.1000E-23	0.1951E-11	0.0000E+00	0.1864E-23	0.8813E-23	0.3229E-12	0.0000E+00	0.9551E-23	0.0000E+00	
0.387	0.1014E-22	0.2690E-22	0.1000E-23	0.1989E-11	0.0000E+00	0.1864E-23	0.8779E-23	0.3407E-12	0.0000E+00	0.1014E-22	0.0000E+00	
0.187	0.1015E-22	0.2850E-22	0.1000E-23	0.2026E-11	0.0000E+00	0.1864E-23	0.8766E-23	0.3532E-12	0.0000E+00	0.1015E-22	0.0000E+00	
-0.013	0.1017E-22	0.2972E-22	0.1000E-23	0.2061E-11	0.0000E+00	0.1864E-23	0.8734E-23	0.3613E-12	0.0000E+00	0.1017E-22	0.0000E+00	

TABLE D-6 Continued

TCLOCK 14459.12 (4.016 HRS)
DT 60.00

GLEVL (KM) -0.013
WAGRID(1) 0.00

Z (KM)	P	CS
4.987	0.5397E+06	0.2498E-04
4.787	0.5540E+06	0.2545E-04
4.587	0.5686E+06	0.2595E-04
4.387	0.5835E+06	0.2647E-04
4.187	0.5987E+06	0.2700E-04
3.987	0.6142E+06	0.2755E-04
3.787	0.6300E+06	0.2812E-04
3.587	0.6462E+06	0.2869E-04
3.387	0.6626E+06	0.2929E-04
3.187	0.6794E+06	0.2989E-04
2.987	0.6966E+06	0.3051E-04
2.787	0.7141E+06	0.3115E-04
2.587	0.7320E+06	0.3182E-04
2.387	0.7502E+06	0.3248E-04
2.187	0.7689E+06	0.3315E-04
1.987	0.7879E+06	0.3384E-04
1.787	0.8073E+06	0.3453E-04
1.587	0.8271E+06	0.3524E-04
1.387	0.8474E+06	0.3595E-04
1.187	0.8680E+06	0.3667E-04
0.987	0.8890E+06	0.3740E-04
0.787	0.9105E+06	0.3815E-04
0.587	0.9324E+06	0.3891E-04
0.387	0.9547E+06	0.3966E-04
0.187	0.9774E+06	0.4039E-04
-0.013	0.1001E+07	0.4109E-04

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