**Description of the
Mountain Cloud Chemistry
Program Version of the PLUVIUS
MOD 5.0 Reactive Storm
Simulation Model**

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July 1987

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SUMMARY

Damage to forest ecosystems on mountains in the eastern United States has prompted a study conducted for the U.S. Environmental Protection Agency's Mountain Cloud Chemistry Program (MCCP). This study has led to the development of a numerical model called MCCP PLUVIUS, which has been used to investigate the chemical transformations and cloud droplet deposition in shallow, non-precipitating orographic clouds.

The MCCP PLUVIUS model was developed as a specialized version of the existing PLUVIUS MOD 5.0 reactive storm model. It is capable of simulating aerosol scavenging, nonreactive gas scavenging, aqueous phase SO_2 reactions, and cloud water deposition. A description of the new model is provided along with information on model inputs and outputs, as well as suggestions for its further development. The MCCP PLUVIUS incorporates a new method to determine the depth of the layer of air which flows over a mountaintop to produce an orographic cloud event. It provides a new method for calculating hydrogen ion concentrations, and provides updated expressions and values for solubility, dissociation and reaction rate constants.

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1.0 INTRODUCTION

The U.S. Environmental Protection Agency (EPA) has initiated a research program to investigate the causes of forest ecosystem damage on mountains in the eastern United States. One proposed mechanism to explain the damage, which has been observed primarily on mountaintops, is the deposition of acidic cloud droplets on forest vegetation during the frequent orographic cloud events. The purpose of this study, conducted for the EPA's Mountain Cloud Chemistry Program (MCCP), is to develop a customized or specialized version of the PLUVIUS MOD 5.0 reactive storm model that can be used to investigate the chemical transformations and cloud droplet deposition in shallow nonprecipitating orographic clouds at a number of MCCP field measurement sites in eastern North America. These sites include: Whiteface Mountain, New York; Mt. Mitchell, North Carolina; Shenandoah, Virginia; Mt. Moosilauke, New Hampshire; Whitetop Mountain, Virginia; and Mt. Tremblant and Mt. Montmorency in Quebec, Canada. The Canadian sites are operated under separate funding from Canada's Atmospheric Environment Service.

The PLUVIUS MOD 5.0 code (Easter and Hales 1984) is a one-dimensional reactive storm simulation model that can simulate the formation of various types of storm systems and can characterize the behavior of air pollutants as they flow through, react within, and are scavenged or deposited by storms. The MCCP version of this code, called MCCP PLUVIUS, includes the relevant chemical reactions to simulate in-cloud processes leading to chemical transformations and cloud water deposition in shallow, nonprecipitating orographic clouds. These cloud types occur frequently on mountains in the eastern United States. Such orographic cloud events can persist for many hours on a given mountaintop and are characterized by deposition of acidic fog droplets on forest ecosystems. The model is expected to be useful to MCCP participants in evaluating the chemical pathways occurring during such events so that effective meteorological and chemical measurement strategies can be developed or refined. The model will also assist in evaluating the utility of the MCCP data base in future investigations of processes leading to observed chemical and cloud characteristics.

This report is intended to be used in conjunction with the definitive report by Easter and Hales (1984), which provides a complete technical description of the PLUVIUS MOD 5.0 model. To the extent possible, the organization of the present document follows the outline of the earlier report, especially in regard to Example Application 2. Thus, the reader can readily determine the special features of the MCCP version of the code. Rather than repeating what has been previously reported, this document concentrates mainly on the differences between MCCP PLUVIUS and PLUVIUS MOD 5.0, Example Application 2, as described in the Easter and Hales (1984) report.

The MCCP PLUVIUS model incorporates a new method for determining the depth of the layer of air that flows over a mountaintop to produce an orographic cloud event. Following this method, a critical dividing streamline height is determined for the airmass upwind of the mountain barrier using topographic and meteorological data.

The model includes aerosol scavenging, nonreactive gas scavenging, aqueous phase SO_2 reactions, and deposition of cloud water. Thirty chemical and water species in various phases are carried as dependent variables in simulations with MCCP PLUVIUS. The model includes updated expressions and values for solubility, dissociation, and reaction rate constants. Expressions for hydroxymethanesulfonate (HMSA) formation and dissociation have been added, and SO_2 oxidation reaction expressions updated, as well. A new Class III subroutine (HIONCALC) was developed for calculating hydrogen ion concentrations, as an alternative to the original empirical method.

The report contains a brief description of the model's governing equations, boundary conditions, and computer code characteristics. This description is followed by an explanation of the parameterizations of the meteorology involved in the creation and maintenance of an orographic cloud, the chemical transformations occurring within the cloud, and the cloud water deposition at the base of the cloud. Model inputs and outputs are summarized through the presentation of a sample (or baseline) case, and suggestions are made for the further development of MCCP PLUVIUS to provide improved simulations of orographic cloud events.

2.0 GOVERNING EQUATIONS, CODE CHARACTERISTICS, AND BOUNDARY CONDITIONS

The MCCP PLUVIUS code numerically approximates solutions to the conservation equations for energy, water species, and pollutant species. Thus, it models water condensation, pollutant transport, gas and aerosol scavenging, aqueous chemical reactions, and associated phenomena as simultaneously occurring events.

The governing material and energy balance equations for MCCP PLUVIUS are the same as for the original PLUVIUS MOD 5.0 model. The theoretical derivations of these equations and boundary conditions are given in Chapter 2 of Easter and Hales (1984); interested readers are referred to this document for detailed information.

Code characteristics of MCCP PLUVIUS are also the same as in the original model. New users of MCCP PLUVIUS are urged to read the overview of initial rules and conventions, logical flow, data input, modular construction, and zero-dimensional facility given in Chapter 3 of Easter and Hales (1984). The two basic classes of dependent variables handled by the model are computed and constrained variables. Computed variables are calculated by the code's finite differencing procedure, while constrained variables are calculated via other relationships (steady-state conditions, solubility constraints, etc.). The user must specify in the input data file which variables are computed and which are constrained.

Subroutines are categorized according to their function within the modular construction of PLUVIUS:

- Class I Subroutines. Subroutines that are essential for basic operation of the code. In the MCCP version of PLUVIUS, we have customized the Class I subroutines to address the problems of chemistry and deposition in shallow, nonprecipitating orographic clouds. In the event that the user wishes to modify any of the Class I subroutines, these modular subroutines may be replaced.
- Class II Subroutines. Subroutines that are essential for basic operation of the code and, in general, should be left unchanged by the user. The main PLUVIUS program, which directly or indirectly calls all of the other subroutines, is included with the Class II subroutines.

- Class III Subroutines. Additional subroutines that are application specific (not essential for basic operation of the code) and supplied by the user (includes all subroutines that are submodules of Class I subroutines).

Subroutines in each of these classes for MCCP PLUVIUS are described in the example application given in Chapter 3 of this report. Users should pay particular attention to Class I and III subroutines, as it is through these modules that the chemical, physical, and transport processes important to a particular application are modeled.

Temperatures, water species, and chemical species in the MCCP PLUVIUS model, as in earlier versions, are specified by a numerical value of the species index in the array C(I,K) where I is the vertical grid point at the current time step and K is the index number assigned to the species. The values of the dependent variables are transferred to a one-dimensional array, CNN(K), during the integration of the generation component of the mass balance equation at each vertical grid point. A species location variable is assigned to each species number in the SETUP subroutine and passed among the various subroutines through the LOCATN common block. This technique has been found to be helpful when dealing with multicomponent systems.

Units employed consistently throughout the code are

concentrations	mol cm^{-3}
length	cm
temperature	K
time	s
pressure	dynes cm^{-2}
energy	ergs

Because of the nature of the governing equations, MCCP PLUVIUS requires boundary conditions at both the top and the bottom of the computational grid. All boundary conditions are set via a user-supplied subroutine. In general, most species have flux-specified top and bottom boundary conditions. In many cases, except for species that deposit from the grid, these boundary conditions are set to zero to describe an impermeable barrier.

3.0 DESCRIPTION OF THE MCCP VERSION OF PLUVIUS

3.1 ORIENTATION

This chapter provides a description of the MCCP version of PLUVIUS and illustrates how the model is used to simulate a cloud event with in-cloud reaction and cloud water deposition. Parameterizations were chosen to simulate a "typical" case at the Mt. Mitchell MCCP observation site. For this specific example, some meteorological data from the August 30-31, 1986, cloud event were used.

The example simulates a column of clear air containing gaseous and aerosol pollutants, which is initialized on the upwind side of the mountain with specific vertical profiles of water vapor, temperature, pressure, and chemical species concentrations. As the event progresses, the column is carried up the mountain with the horizontal velocity of the approaching air flow. The air flow is assumed to be constant with height. The instantaneous vertical velocity of the column is calculated based on the slope of the mountain surface and the strength of the approach flow. As the air is forced up the mountain, it is lifted and cooled. If sufficient water vapor was present in the initial column, the cooling resulting from lifting causes a cloud to form as water vapor condenses on available cloud condensation nuclei. Further lifting increases the cloud water concentrations until the column reaches the summit of the mountain. Descent of the column on the lee side of the mountain causes warming and evaporation of the cloud droplets until, at a certain altitude, the cloud completely dissipates and the column contains clear air with no liquid water.

The MCCP PLUVIUS model simulates chemical reactions and transformations in the moving column, as well as deposition of cloud water and chemical species in cloud water at the base of the column. When the column contains cloudy air, transformations are simulated by a host of processes that depend on the chemical species present and their solubilities and reactions in the aqueous phase. Major pollutant species that are possible contributors to forest damage are included in the model in their relevant phases. The MCCP PLUVIUS model includes the cloud formation mechanisms and chemical processes in highly parameterized forms. These parameterizations and their derivations will be

discussed in detail in Sections 3.2 and 3.3. The next sections describe the input data for the simulation along with descriptions of the Class I, II, and III subroutines used in this version of the PLUVIUS model. The final section describes the model output and interpretation of the output for this example cloud event.

3.2 METEOROLOGICAL PARAMETERIZATIONS

The MCCP version of PLUVIUS requires several meteorologically related inputs. These inputs include wind speed and temperature profiles, a mathematical description of the dividing streamline, and parameters specifying cloud water deposition. Examples used to describe the procedure for obtaining and implementing these inputs are generic and do not necessarily represent an actual event. The MCCP Mt. Mitchell site will be used for illustrative purposes.

3.2.1 Upper-Level Wind Speed and Temperature

Although the MCCP field program at Mt. Mitchell includes some meteorological measurements at two locations (Mt. Gibbs and Commissary Ridge), neither site provides vertical soundings of wind speed, wind direction, temperature, and dew point. The nearest sources of sounding information come from surrounding National Weather Service (NWS) stations that release rawinsondes every 12 h (0000 Greenwich Mean Time (GMT) and 1200 GMT). The closest NWS rawinsonde stations relative to Mt. Mitchell are Huntington, West Virginia (HTS); Greensboro, North Carolina (GSO); Athens, Georgia (AHN); and Nashville, Tennessee (BNA) (Figure 1). These stations are situated north, east, south, and west of Mt. Mitchell, respectively, at distances of 230 to 400 km. A representative sounding may be chosen by determining which of the four stations mentioned above is upwind from Mt. Mitchell. For example, during a Mt. Mitchell cloud event on August 31, 1986, wind directions at the MCCP meteorological sites were from the east-southeast. The closest upwind NWS rawinsonde station would be Greensboro, North Carolina. Assuming an event began at approximately 1900 eastern standard time (0000 GMT), the 0000 GMT August 31 rawinsonde sounding at Greensboro, North Carolina, should be chosen as the most representative sounding for Mt. Mitchell (Figure 2).

AHN	Athens, GA
ALB	Albany, NY
AYS	Waycross, GA
BNA	Nashville, TN
BUF	Buffalo, NY
CAR	Caribou, ME
CHH	Chatham, MA
CHS	Charleston, SC
DAY	Dayton, OH
FNT	Flint, MI
GRB	Green Bay, WI
GSO	Greensboro, NC
HAT	Hatteras, NC
HTS	Huntington, WV
IAD	Washington, DC
JAN	Jackson, MS
JFK	New York, NY
MGM	Montgomery, AL
MIA	Miami, FL
PIA	Peoria, IL
PIT	Pittsburgh, PA
PWM	Portland, ME
SLO	Salem, IL
SSM	Sault Ste Marie, MI
TPA	Tampa, FL
WAL	Wallops Flight Center

FIGURE 1. National Weather Service Rawinsonde Stations in the Eastern United States

FIGURE 2. 0000 GMT, August 31, 1986, Rawinsonde Sounding, Greensboro, North Carolina. Solid line - air temperature; dotted line - dew point temperature.

This particular sounding indicates a moist layer of air between approximately 1100 m MSL and 1800 m MSL. If a parcel of air is lifted from the 1100-m level, the parcel will reach its lifting condensation level (LCL) after only 100 m of ascent and will yield a cloud base of approximately 1200-m MSL. This cloud base height is not consistent with the orographic cloud base height usually observed at Mt. Mitchell (approximately 1600- to 1800-m MSL). Ascent of the entire deep column, initiated at Greensboro and continued up the terrain profile of Mt. Mitchell, would result in a very deep orographic cloud that is not representative of the shallow, nonprecipitating, near-steady-state cloud systems investigated in the MCCP program. The physics of the observed cloud systems is not well represented by lifting a deep, moist column up the entire mountain barrier. In fact, energy requirements are such that air flowing over a mountain barrier often originates in the first few

hundred meters below the summit. Under these circumstances, the mountain acts as an insurmountable barrier to air originating below this level. This level is called the height of the "dividing streamline." Air below the level of the dividing streamline is blocked by the mountain barrier and flow diverges around the sides of the mountain rather than ascending over the mountain. The depth of the layer that can be lifted over the mountain barrier depends on the height of the mountain and the characteristics of the approaching air-mass--specifically, the stability of the approaching airmass and its wind velocity. A simple means of estimating this flow depth is described in the following section.

3.2.2 The Dividing Streamline Concept

The dividing streamline concept has been frequently used in applied meteorology, particularly to determine plume impaction on elevated landforms. This concept is based on energy conservation relationships for atmospheric flows. The height of the dividing streamline is computed from the vertical profiles of temperature and wind velocity, as well as the height of a topographic obstacle, such as a ridge or an isolated mountain (Sheppard 1956). As a starting point, it is useful to define the meteorological variables used to compute the dividing streamline.

The potential temperature of the atmosphere, θ , is defined by

$$\theta = T \left(\frac{p_{00}}{p} \right)^{R/c_p} \quad (1)$$

where T is the absolute temperature, p is the pressure and p_{00} is a reference pressure, usually 1000 mb or 10^5 Pa. R and c_p are the gas constant and constant pressure specific heat of dry air per unit mass, respectively. If large-scale atmospheric motion is adiabatic and reversible, θ is conserved following the motion of an air parcel. Conservation of potential temperature is a good first approximation for this study. If θ increases with height, the atmosphere is said to be stably stratified. Any displacement of a parcel from its equilibrium level (where the parcel's potential temperature is equal to that of its environment) will create a force that opposes the displacement. This force can be approximated by

$$F = \frac{g}{\bar{\theta}} (\theta_s - \theta_p) \quad (2)$$

where F is the force per unit mass, θ_p is the parcel potential temperature, θ_s is the potential temperature of the surroundings, and g is the gravitational acceleration. If it is assumed that 1) the potential temperature increases with height at a constant rate; 2) $(\theta_s - \theta_p) \ll \theta_s$; and 3) the parcel's equilibrium position is z_0 , then Equation (2) can be approximated as

$$F = N^2 (z - z_0) \quad (3)$$

with

$$N^2 = \frac{g}{\bar{\theta}} \frac{\partial \theta}{\partial z} \quad (4)$$

where $\bar{\theta}$ is the average potential temperature over the interval. The quantity N is called the Brunt-Vaisalla frequency. It is the frequency at which a linear internal gravity wave oscillates in a stratified atmosphere. Using Equation (3), the potential energy, P , gained by lifting a parcel against a stratified environment is

$$P(\Delta z) = \int_{\Delta z' = 0}^{\Delta z' = \Delta z} N^2 \Delta z \, d\Delta z' \quad (5)$$

where $\Delta z = (z - z_0)$.

Figure 3 shows the dividing streamline conceptually. Airflow impinging on an infinite, two-dimensional barrier of height h is divided into two regions: a lower one where the airflow is blocked and an upper one where the air flows over the barrier. The dividing streamline separates these two regions and may be thought of as an air parcel trajectory that is tangent to the crest of the barrier. The elevation h_c of this trajectory at a location far enough upwind that it is not affected by the barrier, is the object of this analysis.

FIGURE 3. Schematic Representation of Flow Over a Two-Dimensional Barrier with a Stagnant Region of Blocked Flow Below the Dividing Streamline

The kinetic energy, E , per unit mass of a parcel is given by

$$E = \frac{u^2}{2} \quad (6)$$

where u is the parcel wind speed. A key assumption in the dividing streamline analysis is that air parcels lose kinetic energy at the same rate that they gain potential energy. The air parcels in the blocked flow region contain insufficient kinetic energy to allow them to be lifted over the barrier. The parcels following the dividing streamline have the critical amount of kinetic energy to reach the peak of the barrier. To find h_c , the kinetic energy of a parcel must be greater than or equal to the potential energy gained by lifting the parcel to the elevation of the crest. In the simplest case, the speed of the approaching wind, u , and N are constant with height. If the gain in

potential energy is balanced by the loss in kinetic energy, h_c can be calculated from the relation

$$\frac{N^2 (h - h_c)^2}{2} = \frac{u^2}{2} \quad (7)$$

or, more simply,

$$h_c = h (1 - F_r) \quad (8)$$

where F_r is the internal Froude number, which is defined by

$$F_r = \frac{u}{Nh} \quad (9)$$

To obtain Equation (8), it was assumed that air parcels reach the barrier crest with zero kinetic energy. This relation was found to be valid in experimental studies of flow over three-dimensional hills by Hunt and Snyder (1980).

In most cases, however, both u and N vary with height. In this situation, Equation (5) must be integrated from the height of the mountain crest, h , downward until the potential energy equals the kinetic energy of the flow at that level. Although the potential energy is computed from the integral defined by Equation (5), the kinetic energy is computed solely from the velocity at a given level. The elevation where these balance is h_c . This calculation can be easily performed numerically from digitized sounding data (Spangler 1987). Note that these simple relationships do not account for other processes, such as wave effects and atmospheric moisture, on the computation of h_c , but they do provide an adequate approximation for the types of analyses performed in this study.

To calculate the dividing streamline height, divide the sounding, from the ground level to the height of the mountain, into layers that have both uniform lapse rate and wind speed. To perform this calculation, values of u , $\Delta\theta$, and Δz are defined for each of these layers, while values of θ and p are needed for

the levels separating the layers. (Figure 4 shows this conceptually.) A discrete form of Equation (5) can then be developed from this analysis using the following relationships:

$${}_i\theta_{i+1} = {}_iT_{i+1} \left(\frac{1000}{{}_iP_{i+1}} \right)^{.286} \quad (10)$$

$$\bar{\theta}_i = \frac{{}_{i-1}\theta_i + {}_i\theta_{i+1}}{2} \quad (11)$$

$$\Delta h_i = h - {}_iZ_{i+1} \quad (12)$$

$$\Delta z_i = {}_iZ_{i+1} - {}_{i-1}Z_i \quad (13)$$

$$N_i = \frac{g}{\bar{\theta}_i} \frac{{}_i\theta_{i+1} - {}_{i-1}\theta_i}{\Delta z_i} \quad (14)$$

$$P_n = \frac{1}{2} \sum_{i=1}^n N_i^2 \Delta z_i^2 \quad (15)$$

$$E_n = \frac{U_n^2}{2} \quad (16)$$

To calculate the elevation of the dividing streamline, the value of k must be determined such that

$$P_{k-1} < E_k < P_k \quad (17)$$

It is possible that the value of k will not be unique because of variable atmospheric structure, particularly in the wind profile. In this case, the highest value of k that satisfies Equation (17) should be used. Once k is

FIGURE 4. Schematic Diagram of Discrete Layers for Dividing Streamline Evaluation Procedure

determined, the dividing streamline elevation can then be calculated from the interpolation formula

$$h_c = h - \left[\Delta h_{k-1} + \left(\frac{E_k - P_{k-1}}{P_k - P_{k-1}} \right) \Delta z_k \right] \quad (18)$$

An example of this analysis for the case of Mt. Mitchell (peak elevation 2037-m MSL) follows. Figure 2 shows the resulting six layers of uniform lapse rate and wind speed for the 0000 GMT, August 31, 1986, Greensboro, North Carolina. For illustrative purposes, it was assumed that the observed winds were from 120° true north at 7.5 m s^{-1} and do not vary with height. The actual windspeeds in the Greensboro sounding were about 5 m s^{-1} , but observed values at Mt. Mitchell on the same date were closer to 10 m s^{-1} . An averaged value was believed to be more representative of conditions closer to the mountain. Table 1 displays the parameters needed for this case.

Table 2 displays the results of the calculations of kinetic and potential energies to determine the dividing streamline elevation. In this example,

TABLE 1. Parameters Computed for Example Dividing Streamline Calculation

Layer	Levels	z (m MSL)	Δz (m)	Δh (m)	p (mb)	T (°C)	θ (K)	$\Delta\theta$ (K)	N_1 (s ⁻¹)	U (m s ⁻¹)
0										
	0-1	2037			807	10.1	301.2			
1			167	167				1.5	.018	7.5
	1-2	1870			823	10.3	299.6			
2			690	857				4.5	.015	7.5
	2-3	1180			894	12.7	295.1			
3			50	907				0.1	.008	7.5
	3-4	1130			900	13.1	295.0			
4			290	1197				2.1	.016	7.5
	4-5	840			931	13.9	292.9			
5			510	1707				0.1	.003	7.5
	5-6	330			988	18.6	292.8			
6			50	1757				0.3	.014	7.5
		280			995	18.9	292.5			

k=2; therefore, the dividing streamline lies within layer 2. From Equation (18), the dividing streamline elevation can be evaluated as

$$h_c = 2037 \text{ m} - \left[167 \text{ m} + \frac{28.1 \text{ m}^2 \text{ s}^{-2} - 4.5 \text{ m}^2 \text{ s}^{-2}}{58.1 \text{ m}^2 \text{ s}^{-2} - 4.5 \text{ m}^2 \text{ s}^{-2}} 690 \text{ m} \right] = 1566 \text{ m}$$

Therefore, airflow approaching Mt. Mitchell at elevations below 1566 m will not pass over Mt. Mitchell. Air above 1566 m will contain sufficient kinetic energy to be lifted over Mt. Mitchell.

TABLE 2. Calculated Kinetic and Potential Energies for the Example Dividing Streamline Calculation

Layer	Δh (m)	Δz (m)	$\frac{P}{s^2}$ (m ² s ⁻²)	$\frac{E}{s^2}$ (m ² s ⁻²)
1	167	167	4.5	28.1
2	857	690	58.1	28.1
3	907	50	58.2	28.1
4	1197	290	68.9	28.1
5	1707	510	70.1	28.1
6	1757	50	70.3	28.1

As shown in Figure 2, the dividing streamline rises from elevation h_c upwind of the mountain to become tangent to the mountain at its crest. To account for the parcel trajectories, which rise more slowly than the underlying surface, we may define the dividing streamline as the surface along which a column is lifted to form the orographic cloud. To accomplish this lifting in the model, we must approximate the shape of the dividing streamline by a simple mathematical expression so that the rate of lifting and consequent rate of condensation in the cloud can be calculated. We must then determine the initial temperature and moisture profiles in a column based at the critical dividing streamline height upwind of the mountain. We approximate the height of the dividing streamline by the Gaussian function given as

$$Z(y) = h_c + (h - h_c) \exp\left[-0.5 \left(\frac{y}{\sigma_y}\right)^2\right] \quad (19)$$

where y is the horizontal distance from the mountain crest and σ_y is the standard deviation of the Gaussian function. The value of σ_y may be adjusted by the model user so that the Gaussian function fits the actual mountain profile well near the mountain top. For purposes of illustration, we might arbitrarily define σ_y to be the actual mountain half-width at the height of the lifting condensation level. Equation (19) is appropriate for the example we investigated where $h_c = 1566$ m and $h - h_c = 471$ m. The numerical values of parameters in Equation (19) will change with the wind, temperature, and dew point profiles on any given day, and the analysis must be repeated as meteorological conditions change.

The MCCP PLUVIUS model is initialized upwind of the mountain. In our methodology, we consider the column's base to be located on the dividing streamline at the upwind distance where the height of the dividing streamline is $h_c + 0.1$ m. The column is assigned initial temperature and dew point profiles from the nearest appropriate rawinsonde sounding. The simulation of orographic cloud development is accomplished by lifting the initial column up the Gaussian-shaped path of the dividing streamline using an approach wind speed that is independent of height (note that the MCCP version of PLUVIUS, like the MOD 5.0 version, allows the user the option of specifying an approach wind speed

that varies with height). The model user can determine the lifting condensation level for this initial column with a thermodynamic diagram and, from this height, estimate σ_y for Equation (19). The lifting condensation level depends on the humidity profile in the column at model initiation. If the column is initially saturated (i.e., cloudy), the LCL will be at the critical dividing streamline height. If the column is unsaturated, the LCL will occur above the critical dividing streamline height. For a very dry column, ascent of the mountainside may not produce enough cooling to produce condensation, and an orographic cloud will not form. The MCCP PLUVIUS model will calculate the lifting condensation level automatically in every model simulation, but it is necessary to use the thermodynamic diagram before the model run is initiated in order to specify σ_y .

The above methodology provides a means of accounting for atmospheric stability and winds on the formation of orographic clouds on mountain barriers, using observed sounding data upwind of the mountain, and developing a more realistic orographic cloud than other alternative methods.

3.2.3 Cloud Water Deposition

Deposition of cloud water directly to the surface of the earth has been found, in some cases, to be an efficient pathway for transfer of liquid water to the surface (Choularton et al. 1986; Dollard et al. 1983; Fuzzi et al. 1985). Because cloud water can have pollutant concentrations that are an order of magnitude higher than rainwater, even a small amount of cloud water deposition can affect the total wet deposition of acidic species experienced at the surface. Cloud water deposition is even more important at sites that experience frequent events of cloud and fog water deposition. Previous studies (Lovett and Reiners 1982; Lovett 1984) have shown that the majority of cloud droplet deposition at high horizontal wind velocities occurs through inertial impaction. In the MCCP PLUVIUS model, cloud droplet deposition is parameterized using previously reported cloud deposition data as a function of wind speed, based on the work of Lovett (1984):

$$v_d = 7.63 \times 10^{-2} U_a - 1.25 \quad (20)$$

where v_d is the deposition velocity of the cloud in cm s^{-1} , and U_a is the horizontal wind speed in cm s^{-1} . The deposition velocities are used to calculate the lower boundary condition for the pollutant species in the cloud water phases where the flux at the bottom of the computational grid for a species "a", $FB(a)$, is determined as

$$FB(a) = -v_d C(1,a) \quad (21)$$

where $C(1,a)$ is the concentration of species a at the lowest grid point. The lower boundary condition is set to zero when no cloud water exists in the system at the current grid point.

The cloud water deposition is calculated at the base of the moving column. Because the column is transported to the mountaintop along the dividing streamline, the calculated deposition may occur at an elevation different from the actual ground surface. However, at elevations high on the mountaintop, where MCCP measurements are generally made, the height of the dividing streamline approaches the height of the actual topography. The model user is advised, therefore, to consider the calculated cloud water deposition as representing surface deposition on the actual topography at the column's current horizontal position relative to the mountaintop.

3.3 CHEMICAL PARAMETERIZATIONS

The chemistry included in MCCP PLUVIUS is more detailed than the chemistry included in the example applications given in Easter and Hales (1984). Modeled species include SO_2 , O_3 , H_2O_2 , formaldehyde (HCHO), hydroxymethanesulfonate (HMSA), sulfate, nitrate, and ammonium, with the last two species existing in aerosol, gaseous, and aqueous forms. Carbon dioxide (CO_2), a natural atmospheric component, is automatically included in all gas/aqueous-phase partitioning steps. Provision is also made for following other soluble aerosol components through the excess cation and anion variables (KEXCAT2, KEXCAT1, KEXAN1, KEXAN2). Three aqueous-phase reactions involving SO_2 are also modeled; however, no homogenous gas-phase reactions or gas-to-aerosol-particle conversions are included. Table 3 summarizes the 30 dependent variables that are included in the model. Note that, for certain species, the sum of the

TABLE 3. Dependent Variables for MCCP PLUVIUS Example Application

Variable	Species Location Variable	Type
Temperature	KTEMP	Computed
Water Vapor and Cloud Water	KVAPCL	Computed
Cloud Water	KCLOUD	Constrained by Saturation Equilibrium
Sulfate Aerosol	KS04A1	Computed
Sulfate in Cloud Water	KS04C	Computed
SO ₂ in Gas Phase and in Cloud Water	KS02GC	Computed
SO ₂ in Gas Phase	KS02G	Constrained by Solubility Equilibrium
SO ₂ in Cloud Water	KS02C	Constrained by Solubility Equilibrium
Nitrate in Aerosol, in Gas Phase and in Cloud Water	KN03A1GC	Computed
Nitrate Aerosol	KN03A1	Constrained by Partitioning
HNO ₃ in Gas Phase	KN03G	Constrained by Solubility Equilibrium
Nitrate in Cloud Water	KN03C	Constrained by Solubility Equilibrium
Ammonium in Aerosol, in Gas Phase and in Cloud Water	KNH4A1GC	Computed
Ammonium Aerosol	KNH4A1	Constrained by Partitioning
NH ₃ in Gas Phase	KNH4G	Constrained by Solubility Equilibrium
Ammonium in Cloud Water	KNH4C	Constrained by Solubility Equilibrium
H ₂ O ₂ in Gas Phase and in Cloud Water	KH202GC	Computed
H ₂ O ₂ in Gas Phase	KH202G	Constrained by Solubility Equilibrium
H ₂ O ₂ in Cloud Water	KH202C	Constrained by Solubility Equilibrium
Ozone in Gas Phase	KO3	Computed
Formaldehyde in Gas Phase and in Cloud Water	KFORMGC	Computed
Formaldehyde in Gas Phase	KFORMG	Constrained by Solubility Equilibrium
Formaldehyde in Cloud Water	KFORMC	Constrained by Solubility Equilibrium
HMSA in Aerosol	KHMSXA1	Computed
HMSA in Cloud Water	KHMSXC	Computed
Excess cations of Z=2	KEXCAT2	Computed
Excess cations of Z=1	KEXCAT1	Constrained by Empirical Relationship
Excess anions of Z=2	KEXAN2	Constrained by Empirical Relationship
Excess anions of Z=1	KEXAN1	Constrained by Empirical Relationship
H ⁺ in Cloud Water	KHIONC	Constrained by Electroneutrality or Empirical Relationship ^(a)

(a) Electroneutrality constraint imposed if subroutine HIONCALC used; otherwise empirical relationship used. See discussion of subroutine GEN.

gas-phase concentration and cloud-water-associated concentration is treated as a computed variable (e.g., KS02GC, KVAPCL), while the individual concentrations are treated as constrained variables (KS02G, KS02C, etc.). This treatment is possible because the "phases" are in equilibrium and move with the same vertical velocity. Thus, the total number of computed variables is reduced in the model, which reduces the computing time. Other compounds and chemical mechanisms can be included in the example application by specifying additional reactions and species in the appropriate subroutines.

The user needs to understand not only what chemical species and reactions are included in the model, but also how species are transferred among the aerosol, gas, and aqueous phases. Fewer transfer pathways in MCCP PLUVIUS need to be considered compared to the original PLUVIUS MOD 5.0 model because the only condensed water phase currently included is cloud water. Interaction diagrams are useful in illustrating potential pathways; Figures 5 and 6 are interaction diagrams for sulfur and ammonium species, respectively. The sulfur interaction diagram is more complex than that for ammonium because of the potential for aqueous phase SO_2 reactions. The single line connecting SO_2/cloud to $\text{SO}_4^{2-}/\text{cloud}$ represents the irreversible oxidation of dissolved SO_2 to sulfate by ozone or hydrogen peroxide. The two lines connecting SO_2/cloud and HMSA/cloud represent the reversible reaction of dissolved SO_2 and HCHO to form HMSA. The lines between SO_2/cloud and SO_2/gas represent mass transfer, while the lines between $\text{SO}_4^{2-}/\text{cloud}$ and $\text{SO}_4^{2-}/\text{aerosol}$ represent aerosol scavenging and cloud droplet evaporation. Because no aqueous-phase reactions of ammonium ion are included in the model, Figure 6 illustrates the equilibrium mass transfer of NH_3 between the gas and aqueous phases, the scavenging of ammonium-containing aerosols by condensing cloud droplets, and the release of ammonium-

FIGURE 5. Interaction Diagram for Sulfur Species

FIGURE 6. Interaction Diagram for Ammonium Species

containing aerosols by evaporating cloud droplets. Details of aerosol scavenging, nonreactive gas scavenging, and aqueous-phase reactions within the model will now be discussed.

3.3.1 Aerosol Scavenging

In MCCP PLUVIUS, the following species can exist as aerosol particles: sulfate, nitrate, ammonium, HMSA, excess cations of charge 2, excess cations of charge 1, excess anions of charge 2, and excess anions of charge 1. Aerosol particles in MCCP PLUVIUS are assumed to act as cloud condensation nuclei that are totally soluble within the aqueous phase, and therefore, at the instant of cloud formation, all aerosol species are immediately incorporated into the aqueous phase. Such an assumption is a good approximation for ammonium nitrate and ammonium sulfate aerosols, as these water-soluble compounds are known to be effective cloud condensation nuclei (Stelson et al. 1984). When the cloud evaporates, aerosol particles are immediately reinjected into the clear air. For species, such as ammonium and nitrate, that can exist either as aerosol particles or gases (NH_3 , HNO_3), the ratio of reinjected aerosol to reinjected gas is set equal to the ratio of aerosol to gas in the initial conditions.

In this example application, it is assumed that once a cloud evaporates, all HMSA formed by the aqueous-phase reaction of SO_2 and HCHO is reinjected as HMSA aerosol. It is not known if this assumption is valid because the existence of HMSA in fog and rainwater samples is a relatively recent finding

(Munger et al. 1984; Chapman 1986). We are not aware of HMSA being found in aerosol samples, although sampling difficulties associated with analyzing this compound do not make this surprising. Based on current information, it appears equally plausible to have the model dissociate HMSA back into SO_2 and HCHO as the cloud evaporates. However, using a zero HMSA input concentration and treating the formed HMSA as an injected aerosol facilitates assessment of the importance of this compound in aqueous-phase sulfur chemistry. For this reason, HMSA is treated as a stable compound during cloud evaporation in the example application.

Users must exercise caution when assigning initial conditions if they intend to have the model actually calculate the equilibrium hydrogen ion concentration (i.e., if they intend to employ subroutine HIONCALC rather than empirical relationships). Differences in input aerosol anion and cation concentrations (on an equivalent basis) will affect the charge balance within the aqueous phase and thus affect the calculated equilibrium pH. For example, if a user specifies a certain input for nitrate aerosol but fails to "neutralize" the aerosol by including nonzero inputs for ammonium or cation aerosol species, the resulting aqueous phase NO_3^- will be charge balanced with hydrogen ion. In essence, the user has unintentionally turned nitrate aerosol scavenging into additional HNO_3 scavenging. This situation can be avoided by the user deciding a priori what percentage of input aerosol is to exist in neutralized form and adjusting input concentrations for the various aerosols (i.e., inputs for $\text{KNH}_4\text{A1}$, $\text{KNO}_3\text{A1}$, KS04A1 , KHMSX1 , KEXCAT2 , KEXCAT1 , KEXAN1 , and KEXAN2) to achieve this percentage.

Nonreactive species that are not explicitly followed in MCCP PLUVIUS, but which may be important to the solution charge balance (and thus affect the equilibrium H^+ concentration), should be incorporated via the excess cation and anion variables. If, for example, in a case-study application, it is known that scavenging of Ca^{2+} neutralizes a certain amount of acidity, the Ca^{2+} data can be used in selecting an input for the KEXCAT2 variable. In this situation, a charge balancing input for an anion aerosol species does not need to be specified. Information on Cl^- , PO_4^{3-} , Na^+ , K^+ , and Mg^{2+} can be incorporated similarly.

3.3.2 Nonreactive Gas Scavenging

In MCCP PLUVIUS, it is assumed that the rate of mass transfer from the gas to the liquid phase is much faster than the rate of any liquid phase reactions so that equilibrium scavenging conditions exist. This assumption was demonstrated to be valid for cloud water droplets with their high surface-to-volume ratio for normal ranges of atmospheric pollutants (Schwartz 1984). However, for unusual (and probably unrealistic) input conditions that lead to very rapid aqueous-phase reaction rates, the equilibrium scavenging assumption may no longer hold. As an example, consider a situation where an input concentration of the highly soluble oxidant H_2O_2 is 20 times greater than that of the moderately soluble SO_2 . Under such conditions, it is possible that the conversion rate of SO_2 to sulfate will be limited by the mass transfer rate of SO_2 from the gas to the aqueous phase. Users should avoid using MCCP PLUVIUS for modeling situations where equilibrium scavenging conditions do not exist, as model results will be invalid. Excellent reviews of mass-transport limited situations and the calculation of various characteristic time constants needed to evaluate such situations are given in Schwartz (1984) and Schwartz and Freiberg (1981). Users concerned that a given application may be mass-transport limited are urged to consult these articles.

Parameterizations of solubility constants (K_0) and equilibrium constants (K_1 , K_2) for the various gases and aqueous species considered in MCCP PLUVIUS are summarized in Tables 4 and 5, respectively. Note that a composite Henry's Law/dissociation constant is used for both HNO_3 and NH_3 (i.e., it is assumed that concentrations of the species $\text{HNO}_3(\text{aq})$ and $\text{NH}_3(\text{aq})$ are negligible). This assumption is valid for $0.8 < \text{pH} < 7.2$ and thus covers the pH range normally encountered in acid deposition work. At pH 0.8, the concentration of $\text{HNO}_3(\text{aq})$ is approximately 1% of the total dissolved nitrate (defined as $[\text{HNO}_3(\text{aq})] + [\text{NO}_3^-]$), while at pH 7.2 the concentration of $\text{NH}_3(\text{aq})$ is approximately 1% of the total dissolved ammonium (defined as $[\text{NH}_3(\text{aq})] + [\text{NH}_4^+]$).

3.3.3 Aqueous Phase SO_2 Reactions

Three chemical reactions involving dissolved SO_2 are included in MCCP PLUVIUS. Two reactions are oxidation reactions involving O_3 and H_2O_2 that convert dissolved SO_2 into dissolved SO_4^{2-} . The third is the reaction of dissolved SO_2 and dissolved HCHO to form the adduct HMSA. Because the latter

TABLE 4. Solubility Constants Used in Model Calculations.₁
(Units for solubility constants are mol L⁻¹ atm⁻¹,
while units for composite solubility/dissociation
constants are as indicated.)

Solubility Process	Solubility Constant	Ref.
SO ₂ (g) ⇌ SO ₂ (aq)	[SO ₂ (aq)]/[SO ₂ (g)] = exp(-10.25 + 3121.7/T)	(a)
CO ₂ (g) ⇌ CO ₂ (aq)	[CO ₂ (aq)]/[CO ₂ (g)] = antilog (-14.018 + 2385.7/T + .015264 x T)	(b)
HNO ₃ (g) ⇌ H ⁺ + NO ₃ ⁻	[H ⁺] [NO ₃ ⁻]/[HNO ₃ (g)] = exp(4474.3/T) mol ² L ⁻² atm ⁻¹	(c)
NH ₃ (g) ⇌ NH ₄ ⁺ + OH ⁻	[OH ⁻] [NH ₄ ⁺]/[NH ₃ (g)] = 12.187 K _w /T antilog (-1.60 + 4207.6/T) mol ² L ⁻² atm ⁻¹	(d)
H ₂ O ₂ (g) ⇌ H ₂ O ₂ (aq)	[H ₂ O ₂ (aq)]/[H ₂ O ₂ (g)] = exp(-12.24 + 6981.6/T)	(e)
O ₃ (g) ⇌ O ₃ (aq)	[O ₃ (aq)]/[O ₃ (g)] = 1.402 x 10 ⁻⁵ exp(2013.1/T)	(f)
HCHO(g) ⇌ HCHO(aq)	[HCHO(aq)]/[HCHO(g)] = exp(-12.71 + 6425/T)	(g)

(a) Hales and Sutter 1973; Johnstone and Leppla 1934.

(b) Harned and Davis 1943.

(c) Schwartz and White 1981; Wagman et al. 1968.

(d) Hales and Drewes 1979; K_w from Table 5.

(e) Martin and Damschen 1981, as derived from Scatchard et al. 1952.

(f) Wagman et al. 1968.

(g) Chameides and Davis 1983, as derived from Wagman et al. 1968.

TABLE 5. Aqueous Equilibrium Expressions Used in Model Calculations. (Units are mol L⁻¹ unless otherwise noted.)

Equilibrium Process	Equilibrium Constant	Ref.
$\text{SO}_2(\text{aq}) \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	$[\text{H}^+][\text{HSO}_3^-]/[\text{SO}_2(\text{aq})]$ $= \exp(-10.965 + 1972.4/T)$	(a)
$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	$[\text{H}^+][\text{SO}_3^{2-}]/[\text{HSO}_3^-]$ $= \exp(-23.14 + 1954.7/T)$	(b)
$\text{CO}_2(\text{aq}) \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	$[\text{H}^+][\text{HCO}_3^-]/[\text{CO}_2(\text{aq})] = \text{antilog}$ $(14.8435 - 3404.71/T - 0.032786 \times T)$	(c)
$\text{HCO}_3^- \rightleftharpoons \text{H}^+ + \text{CO}_3^{2-}$	$[\text{H}^+][\text{CO}_3^{2-}]/[\text{HCO}_3^-] = \text{antilog}$ $(6.498 - 2902.39/T - 0.02379 \times T)$	(c)
$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	$[\text{H}^+][\text{OH}^-] = K_w = \text{antilog}$ $(-4.098 - 3245.2/T + 2.2362 \times 10^5/T^2$ $- 3.984 \times 10^7/T^3) (\text{mol L}^{-1})^2$	(d)
$\text{S(IV)} + \text{HCHO}(\text{aq}) \rightleftharpoons \text{HMSA}$	$[\text{S(IV)}][\text{HCHO}(\text{aq})]/[\text{HMSA}] = K_{\text{HMSA}}$ $= \exp(6573/T - 6.71)$	(e)

- (a) Hales and Sutter 1973; Johnstone and Leppla 1934.
 (b) Weast 1984; Beilke and Gravenhorst 1978.
 (c) Harned and Davis 1943.
 (d) Weast 1984.
 (e) Deister et al. 1986.

is an addition reaction, no change in oxidation state occurs and the HMSA sulfur remains in the +4 oxidation state. Table 6 summarizes the reactions and rate constants used in MCCP PLUVIUS. The term S(IV) refers to all forms of SO_2 in the aqueous phase, so

$$[\text{S(IV)}] = [\text{SO}_2(\text{aq})] + [\text{HSO}_3^-] + [\text{SO}_3^{2-}] \quad (22)$$

3.4 INPUT DATA

Input data for this example application are given in Table 7. The input file is similar in form to that reported in the PLUVIUS MOD 5.0 User's Guide (Easter and Hales 1984), with the addition of some variables at the end. Most of the initial data is read by the PLUVIUS Class II main program in the section that is reproduced in Table 8. The first line of the input file is the run title (up to 80 characters) that is printed on the ASCII output file. In the second line, the number of computed and constrained variables are defined (NCOMP and NCONST). The following 30 lines define the alphanumeric variable names to be used in the tabulated printout. These variable names correspond to the names given in Table 3. In the next input line, the number of vertical grid points (N) is specified as 26; two diffusion regimes (LTD) are defined; the vertical grid spacing (DZ) is set to 0.02 km; and the elevation of the grid bottom at the beginning of the computation (GLEVL) is set to zero. Because the total extent of the vertical domain is based on both the grid spacing and the number of grid points, these qualities should be changed for each specific application to attain the resolution desired by the user. In the next input line, the model simulation is specified to proceed from time = 0 (TSTART) to time = 1150 s (TSTOP), with an initial time increment of 15 s. The following line specifies 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 a regular time interval printout, set DTPRIN to the desired interval and NPRINT to 0. If NPRINT is positive (and DTPRIN = 0), then the print-out will occur after each set of NPRINT time steps. ITCOLL and DTCOLL control model output to disk file as follows:

TABLE 6. Aqueous Chemical Reactions and Rate Constants Used in the Simulation Model. [Units are mol L⁻¹ for aqueous concentrations and mol L⁻¹ s⁻¹ for reaction rates. S(IV) - O₃ reaction rate must be multiplied by a liquid diffusion rate limiting term (see text).]

Reaction	Reaction Rate	Ref.
$S(IV) + H_2O_2(aq) \rightarrow SO_4^{2-}$	$d[SO_4^{2-}]/dt = \{6.208 \times 10^{14} \exp(-4751.2/T) [H^+] [HSO_3^-] [H_2O_2(aq)]\} / (1 + 13 [H^+])$	(a)
$S(IV) + O_3(aq) \rightarrow SO_4^{2-}$	$d[SO_4^{2-}]/dt = \{2.4 \times 10^4 [SO_2(aq)] + 4.245 \times 10^{13} \exp(-5533.1/T) [HSO_3^-] + 7.376 \times 10^{16} \exp(-5280.5/T) [SO_3^{2-}]\} [O_3(aq)]$	(a)
$S(IV) + HCHO(aq) \rightarrow HMSA$	$d[HMSA]/dt = k_f [S(IV)] [HCHO(aq)]$ $k_f = (a_1 k_1 + a_2 k_2) / (1 + K_h)$ $a_1 = [HSO_3^-] / [S(IV)]$ $a_2 = [SO_3^{2-}] / [S(IV)]$ $k_1 = T \times \exp(10.78 - 2990/T)$ $k_2 = T \times \exp(19.95 - 2460/T)$ $K_h = 1.82 \times 10^3 \exp(-13.56 + 4041.4/T)$	(b)
$HMSA \rightarrow S(IV) + HCHO(aq)$	$d[HMSA]/dt = -k_r [HMSA]$ $k_r = k_f / K_{HMSA}$	(c)

(a) Hoffman and Calvert 1986.

(b) Boyce and Hoffman 1984.

(c) k_f is the forward rate constant from the previous reaction and K_{HMSA} is the S(IV)-HCHO-HMSA equilibrium constant from Table 5.

TABLE 7. Input Data for the Example Application

MCCP EXAMPLE RUN: BASE CASE VALUES

13	17						
TEMP							
VAPCL							
S02-GC							
S04-A1							
S04-C							
N03-A1GC							
NH4-A1GC							
H2O2-GC							
O3-G							
EXCAT-2							
FORM-GC							
HMSX-A1							
HMSX-C							
CLOUD							
EXCAT-1							
HION-C							
S02-G							
S02-C							
H2O2-G							
H2O2-C							
N03-G							
N03-C							
N03-A1							
NH4-G							
NH4-C							
NH4-A1							
FORM-G							
FORM-C							
EXAN-1							
EXAN-2							
26	2	0.2E4	0.0				
	000.	1150.	15.				
0	288.	-1	30.				
1	0	1	1	0	1	1	0
1	1	1		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
1	1	2		0.			
0.84E6		284.15					
2.	2.	3.	1.				
2.	5.	0.4					
70.	1.	2.					
1.	1.	1.					
750.							

TABLE 8. Input Section of the PLUVIUS Class II Main Program

```

C-----
C
C      INPUT SECTION
C-----
      READ (LUNIN,9000) MTITLE
      READ (LUNIN,9010) NCOMP,NCNSTR
      NTOT=NCOMP+NCNSTR
      IF ((NCOMP.GT.NCMAX) .OR. (NTOT.GT.NCTMAX)) STOP 9990
      IF ((NCOMP.LT.1) .OR. (NCNSTR.LT.0)) STOP 9991
      DO K=1,NTOT
        READ (LUNIN,9000) (NAME(LL,K),LL=1,5)
      END DO
      READ (LUNIN,9020) N,LTD,DZ,GLEV
      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,ISETTL,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, TEMPO

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-----

```

ITCOLL = 0 No disk file output.

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

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

For this example, output is printed out to an ASCII file every 288 s and to a disk file every 30 s.

The next input line provides control variables for bypassing a number of subroutines if their corresponding physical relationships are either constant in time or unimportant to the modeling problem at hand. If the value of a bypass variable is set positive, the appropriate subroutines are interrogated at each time step. If the variable is set to zero or a negative value, the related routines are either called once during the initialization stage of the program execution or are bypassed completely, as appropriate. The significance of the bypass variables and their corresponding subroutines are listed in Table 9. Bypass variables IDIFF, ISETTL, and ISHEAR are set to zero in this simulation because the diffusivities do not change during the simulation, settling velocities are zero, and no wind shear exists. The rest of the bypass variables are set to 1 so that the corresponding subroutines are called during every integration step (see Easter and Hales 1984 for a more detailed explanation of the bypass variables). The next 13 lines specify 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 variables to positive values imposes flux-specified conditions. If the variables are set equal to zero, the boundary conditions become concentration-specified (inflow). If the variables 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 often necessary to apply after the advection-diffusion step for species with large settling velocities. A value of 0 for FILFAC turns off the filter. In this example, all top and bottom grid fluxes are determined to be flux-specified and are set to 1. Temperature is specified in diffusion regime 1, and the remaining

TABLE 9. 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
ISE TTL	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

computed variables are specified in diffusion regime 2, since they are all airborne species. All values of FILFAC are set equal to zero as there are no settling velocities for any of the species. In the next line, the initial pressure at the bottom grid point (PRESS0) is set to 0.84×10^6 dynes cm^{-2} and the initial temperature (TEMPO) is set to 284.15 K. The remainder of the input lines are read in from the Class I subroutine, SETUP, in the format specified in this subroutine (see Appendix A for a listing). In the first three of these lines, the initial, upwind mixing ratios of pollutants in the clear air at the dividing streamline level are read in parts per billion (ppb). For this example, ground-level mixing ratios were chosen from values that seemed to be reasonable for the atmosphere on Mt. Mitchell. Input values were based on site observations whenever possible. Input values for variables that were not measured at the site were taken from values reported in the literature. The next input line specifies values for the ratios of the concentrations of the cations with charge +1 and the anions with charges +1 and +2 determined relative to the concentrations of the cations with charge +2. The factors used for these relationships are defined by

$$RCAT1_RCAT2 \equiv C(I,KEXCAT1)/C(I,KEXCAT2) \quad (23)$$

and the input values for these ratios are determined by the degree of neutralization desired (see Section 3.3). The last line of the input file specifies the dividing streamline-level wind speed for the simulation.

The variables that need to be passed among the various MCCP PLUVIUS subroutines in COMMON blocks were merged into an additional file that is incorporated into the subroutines through use of the 'INCLUDE' statement. A listing of this file, PLUVCMN.FOR, is given in Table 10. Many of the arrays are dimensioned through this inclusion based on the specified maximum number of constrained and computed variables and the maximum number of vertical grid points. The logical units for the input and output files (LUNIN and LUNOUT) are also specified in this file. In this example, the input file must be assigned to unit 21 while the output file is written to unit 25.

3.5 CLASS I SUBROUTINES

A short description of each of the Class I subroutines is provided in this section. The discussion concentrates on the differences between MCCP PLUVIUS and PLUVIUS MOD 5.0 Example 2 in Easter and Hales (1984). Complete listings of all of the Class I subroutines can be found in Appendix A.

3.5.1 Subroutine SETUP

In subroutine SETUP, the initial vertical concentration profiles for the dependent and state variables are calculated, the species location variables are specified, and several other control parameters are defined. Initial pollutant concentrations must be stipulated to supply complete arrays of concentrations and temperatures corresponding to time = 0 in the model computation.

The first set of READ statements are used to input values for the initial, upwind mixing ratios of the chemical species used in the model. These values are read from the designated input unit and are in units of ppb. The ratios of the concentrations of the cations with charge +1 and the anion species to the concentration of the cations with charges of +2 are read in. The next READ statement inputs a value for the ground-level wind velocity.

TABLE 10. Listing of MCCP PLUVIUS Common Blocks Held
in the PLUVCMN.FOR Include File

```

PARAMETER ( NZMAX=26 )      ! NO. OF VERTICAL GRID POINTS
PARAMETER ( NCMAX=25 )      ! NO. OF "COMPUTED" VARIABLES
PARAMETER ( NCTMAX=38 )     ! NO. OF COMPUTED+CONSTRAINED VARIABLES

PARAMETER ( NNAMMX= NCTMAX+2 )
PARAMETER ( LUNIN=21, LUNOUT=25 )

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, XVDB, XRGB,
+   ITEMP, IPRESS, ISETTL, IBOUND, IVERT, IFOG, ISHEAR,
+   COUTSD(NZMAX,NCMAX)

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

COMMON /CHEM/ CNN(NCTMAX), GGEN(NCTMAX), GDEC(NCTMAX),
+   CMIN(NCTMAX), DTSAVE(NZMAX), AEROFRACNO3, AEROFRACNH4,
+   RCAT1_CAT2, RAN1_CAT2, RAN2_CAT2

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

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

COMMON /LOCATN/ KTEMP, KVAPCL, KRAIN, KSNOW, KCLOUD,
+   KS02GC, KS02R, KS02S, KS02G, KS02C,
+   KS04A1C, KS04A1, KS04C, KS04R, KS04S,
+   KHIONC, KHIONR, KO3G,
+   KH2O2GC, KH2O2R, KH2O2S, KH2O2G, KH2O2C,
+   KNO3A1GC, KNO3R, KNO3S, KNO3A1, KNO3G, KNO3C,
+   KNH4A1GC, KNH4R, KNH4S, KNH4A1, KNH4G, KNH4C,
+   KEXCAT1, KEXCAT2, KEXAN1, KEXAN2,
+   KFORMGC, KFORMG, KFORMC,
+   KHMSXA1, KHMSXC

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)

```

The first data statement defines the value used for bypassing rain and snow species (set equal to 1 for this version since rain and snow are not currently included in MCCP PLUVIUS). The following statements define the species location variables and values used in the integration routine. The array of values CMIN(K) is used to set minimum concentration values for each species because some of the integration routines are unable to handle values of zero without faulting.

In the first executable statements, the temperature and dew point temperature profiles are set based on initial soundings measured upwind of the event and the initial relative humidity and water vapor plus cloud profile is calculated (see Section 3.2.1). The initial profiles of other species are determined based on a compilation of experimental and modeled profile shapes previously reported in the literature. Species profiles from the SURE experiment (Blumenthal et al. 1984) were used in this compilation as were numerous other sources. From the previously reported profiles, a species-specific profile was calculated based on the "average" profile shape and the input ground concentrations for each species.

3.5.2 Subroutine ADJUST

Subroutine ADJUST calculates a new cloud concentration based on the current temperature and concentration of water at the current grid point.

3.5.3 Subroutine BOUND

In subroutine BOUND, the top boundary conditions are specified to be zero for each chemical species, because transfer across this level is currently unknown but should be small in a stable environment. In addition, for the lower boundary condition, zero flux is specified for gases and aerosols because dry deposition is negligible compared to cloud water deposition. For the cloud phase, an outflow bottom boundary condition is specified to be the product of the concentration and the deposition velocity. The deposition velocity is calculated as a function of the surface wind speed based on a parameterization of literature values. Both the bottom and the top boundary conditions can be easily changed to fit different situations.

3.5.4 Subroutine DIFF

This subroutine sets the vertical eddy diffusivity to $10^5 \text{ cm}^2 \text{ s}^{-1}$ for the temperature, gaseous, aerosol, and cloud regimes. This value was chosen to represent a reasonable value for a moderately stable atmosphere. Different values could be set for each separate regime, if desired.

3.5.5 Subroutine GRDSET

GRDSET sets a uniform vertical spacing for the computational grid. If a greater resolution is desired in a certain region of the vertical grid, this resolution can be changed to proportional spacing following a user-specified input function.

3.5.6 Subroutine SETTLE

Subroutine SETTLE computes the settling velocity for all species. Because there are no rain or snow species in this version, and cloud droplet deposition by impaction is much larger than that by sedimentation for this example, all of the species are calculated with a settling velocity of zero.

3.5.7 Subroutine TIMESP

TIMESP sets the basic integration time step, Δt , based on the maximum vertical velocity of the grid and the grid spacing. Both maximum and minimum values of Δt are specified. These values can be determined by finding the largest Δt (smallest computing time) that can still accurately compute the results.

3.5.8 Subroutine USHEAR

The ratio $URATIO = u^*/U_a$ is set in subroutine USHEAR, where u^* is the wind speed at the reference level, and U_a is the wind speed at the current vertical grid level. In this example, the wind speed is constant with height so that $URATIO(I)$ is equal to 1.0 at all vertical grid points. This specification can be easily changed to incorporate a wind speed that changes with vertical height.

3.5.9 Subroutine VERT

Subroutine VERT calculates the velocity of the grid, where this updraft velocity is driven by the rate of change of the dividing streamline height

with horizontal distance (see Section 3.2.2). For this example, the velocity component relative to the grid has been arbitrarily set to zero, and the change in grid height is given by differentiating the appropriate Gaussian dividing streamline height expression with respect to time. As mentioned in Section 3.2.2, this expression must be changed when the physical conditions (mountain shape, wind speed) change. Because this example assumes no wind shear, the grid vertical velocity is equal to dZ/dt .

3.5.10 Subroutine GEN

GEN computes the generation and decay rates for the computed species, determines pollutant gas/aqueous partitioning, and sets values for the constrained species. In this example application, GEN is the largest of the Class I subroutines; it calls three Class III subroutines (DISSCON, HIONCALC, and DIFLIM03) that will be discussed in detail in Section 3.7. GEN does not require modification for model applications to different sites or conditions.

At the start of GEN, parameters used in calling the Class III subroutines are initialized and local water and temperature variables are defined. By calculating the water vapor saturation concentration, the model determines whether or not a cloud is present. If not, all aqueous-phase concentrations are set to a minimum value (CMIN, defined in subroutine SETUP), aerosol and gas-phase concentrations are established, and a return to the main program is executed. If a cloud is present, a call to DISSCON is made to establish all solubility and dissociation constants. Depending on the value assigned to variable KHCALC at the start of GEN, hydrogen ion concentration in the aqueous phase is determined either by an empirical relationship or by calling subroutine HIONCALC for an explicit calculation. The empirical relationship is derived from MAP3S Precipitation Chemistry Network data (MAP3S/RAINE 1982) and is the same as that used in Example 2 of Easter and Hales (1984). In the example of MCCP PLUVIUS presented here, subroutine HIONCALC is called. Once the aqueous-phase hydrogen ion concentration is determined, gas/aqueous partitioning calculations are performed. Aqueous O_3 concentration is calculated as a temporary variable because ozone has a low solubility and the aqueous level is small compared to that in the gaseous phase. All aerosols are incorporated into the aqueous phase and pollutant aerosol concentrations are set equal to corresponding values in array CMIN(K) (as defined in subroutine SETUP). The pH-

dependent concentrations of the various forms of dissolved SO_2 ($\text{SO}_2(\text{aq})$, HSO_3^- , SO_3^{2-}) are calculated and used in computing aqueous SO_2 reaction rates. Rate expressions and rate constants employed in GEN are summarized in Table 6. Subroutine DIFLIM03 is called in the calculation of the SO_2 - O_3 reaction rate to determine the value of the liquid diffusion rate-limiting term. Finally, net generation and decay terms are calculated for each species.

3.5.11 Subroutines RAIN and SNOW

Subroutines RAIN and SNOW will handle the addition of rain and snow species, if the appropriate value for IWSPEC is specified. These subroutines will be called with a parameter that specifies which values need to be calculated at the current program step. RAIN and SNOW are left as do-nothing subroutines in the current version of the program, because the primary focus of current modeling efforts was cloud droplet chemistry and deposition. We anticipate that future versions of MCCP PLUVIUS will include working subroutines RAIN and SNOW. Calls to these subroutines have been incorporated into the code to facilitate this future work and to aid advanced users who wish to supply their own parameterizations.

3.6 CLASS II SUBROUTINES

As indicated previously, Class II subroutines are essential for basic operation of the code and, in general, should not be modified by the user. (Modify at your own risk!) Computational routines involved in the numerical integrations, thermodynamic routines, and output routines are included in this category. Two minor modifications to the Class II subroutines of PLUVIUS MOD 5.0 were made for the MCCP PLUVIUS version:

1. Subroutine COLLECT has been changed to incorporate a call to subroutine GEN just before writing unaveraged values to a disk file.
2. The error check and step-size increment calculation in subroutine ODEINT has been changed to give slightly less error relaxation.

Listing and additional information on Class II subroutines can be found in Easter and Hales (1984).

3.7 CLASS III SUBROUTINES

MCCP PLUVIUS contains three Class III subroutines: DISSCON, HIONCALC, and DIFLIM03. These subroutines relate to the treatment of aqueous-phase chemistry within the model and all are called by subroutine GEN. Complete listings of these subroutines can be found in Appendix B. No modifications of these subroutines are required for application of MCCP PLUVIUS to different sites or conditions.

3.7.1 Subroutine DISSCON

Subroutine DISSCON calculates the temperature- and pressure-dependent solubility parameters and equilibrium constants for the various species considered within the model. Local temperature and air density are required inputs to the routine. Solubility parameters (also called Henry's Law constants) are labelled as OK0xxx (where the xxx stands for the species name) and are based on the expressions given in Table 4. Conversion factors are applied to produce the solubility parameters in units of $\text{cm}^3 \text{ space L}^{-1} \text{ H}_2\text{O}$. This seemingly awkward unit is useful for calculations in subroutine GEN, since multiplication of OK0xxx terms by gas-phase pollutant concentrations with the standard MCCP PLUVIUS units of $\text{mol cm}^{-3} \text{ space}$ produces aqueous-phase concentrations in $\text{mol L}^{-1} \text{ H}_2\text{O}$. Equilibrium constants involving the first dissociation of an H^+ ion are labelled as DK1xxx, while those involving the second dissociation are labelled as DK2xxx (where the xxx again stands for the species name). All equilibrium constants are in units of $\text{mol L}^{-1} \text{ H}_2\text{O}$, except for the equilibrium constant for water (DKW), which is in $\text{mol}^2 \text{ L}^{-2}$, and are based on the expressions given in Table 5. Various OK0xxx, DK1xxx, DK2xxx products are also determined for computational efficiency in performing the gas/aqueous-phase partitioning calculations in subroutine GEN. Calculations for CO_2 assume a mixing ratio of 330 ppm at 1 atm total pressure, the value commonly given for a standard atmosphere (Weast 1984), with proportional concentrations at other pressures. Calculated values for all solubility parameters and their products are placed in labelled common block DISSCON.

3.7.2 Subroutine HIONCALC

The purpose of subroutine HIONCALC is to answer the following question:

Given a nonequilibrium situation where liquid water containing certain concentrations of cations and anions exists with gases that will dissolve into this liquid water (thereby changing the concentrations of cations and anions), what will be the concentration of hydrogen ion at equilibrium?

HIONCALC iteratively calculates this equilibrium aqueous-phase hydrogen ion concentration to within a user-specified error tolerance via an ion balance approach. Required subroutine inputs include the gas plus cloud concentrations of SO_2 , nitrate and ammonium in mol cm^{-3} space and the aqueous-phase concentrations of the excess anion and cation variables in $\text{mol L}^{-1} \text{H}_2\text{O}$. With an assumed nucleation efficiency equal to unity for all aerosol particles, gas plus cloud concentrations correspond to the total (gas plus cloud plus aerosol) concentrations; thus, species location variables KN03A1GC and KNH4A1GC are used in the call from subroutine GEN. Concentrations of ionic species that do not have a gas-phase analog (e.g., SO_4^{2-} and HMSA) must be added to the appropriate excess anion and cation variables before HIONCALC is called; see, for example, the four lines of code in subroutine GEN just before the "CALL HIONCALC" statement. Other required inputs are temperature, air density, liquid water concentration, the diagnostic variable IOK, and an initial guess for the equilibrium hydrogen ion concentration (HION). On the first call to the subroutine, variable HION is undefined and internally set equal to 2.5×10^{-6} , the pH existing when atmospheric CO_2 is in equilibrium with pure water. On subsequent calls, the input HION value is equal to that calculated during the last subroutine call.

Subroutine HIONCALC uses a standard ion balance approach to determine the equilibrium hydrogen ion concentration. The basic equation being solved is

$$[\text{HSO}_3^-] + [\text{NO}_3^-] + [\text{HCO}_3^-] + [\text{OH}^-] + [\text{KEXAN1}] + 2\{[\text{SO}_3^{2-}] + [\text{CO}_3^{2-}] + [\text{KEXAN2}]\} = [\text{H}^+] + [\text{NH}_4^+] + [\text{KEXCAT1}] + 2[\text{KEXCAT2}] \quad (24)$$

where KEXAN1, KEXAN2, KEXCAT1, and KEXCAT2 are the excess anions and cations of charge 1 and 2. By using the definitions of the solubility and equilibrium constants and their respective numerical expressions, as given in Tables 4

and 5, Equation (24) can be converted into a form where the only unknown is $[H^+]$:

$$A[H^+]^3 + B[H^+]^2 + C[H^+] + D = 0 \quad (25)$$

where $A = 1 + K_{NH3}[NH_3(g)]/K_w \quad (26)$

$$B = [KEXCAT1] + 2[KEXCAT2] - \{[KEXAN1] + 2[KEXAN2]\} \quad (27)$$

$$C = K_{OS02} K_{1S02} [SO_2(g)] + K_{HNO3} [HNO_3(g)] + K_w \\ + K_{OC02} K_{1C02} [CO_2(g)] \quad (28)$$

$$D = 2 (K_{OS02} K_{1S02} K_{2S02} [SO_2(g)] + K_{OC02} K_{1C02} K_{2C02} [CO_2(g)]) \quad (29)$$

When $[H^+]$ is greater than $0.0001 \text{ mol L}^{-1}$, the "D" term in Equation (25) can be neglected and the cubic relationship reduced to a quadratic equation.

HIONCALC uses the value of HION passed in the subroutine call list as its first "guess" in determining the gas/aqueous-phase partitioning of the various species. Gas-phase concentrations are then used in calculating the A, C, and D coefficients, and Equation (25) is employed to refine the estimate of the equilibrium $[H^+]$. During these calculations, the "D" term is omitted for $[H^+] > 0.0001 \text{ mol L}^{-1}$ and the quadratic equation is solved explicitly. For $[H^+] < 0.0001 \text{ mol L}^{-1}$, the "D" term is included and 10 iterations of Newton's method are used to find the approximate value of the equilibrium hydrogen ion concentration. This value is then further refined by substituting calculated values back into Equation (24) and using a modified Newton's method to iteratively approach the $[H^+]$ for which the ion balance comes as close to zero as possible. The iteration stops when successive passes produce ion balance errors of opposite sign (implying that true solution must be between the last two calculated values of $[H^+]$) and the absolute difference between the two calculated $[H^+]$ s is less than the user-specified error tolerance multiplied by the first of these two calculated $[H^+]$ s. This second refinement process is especially important when the equilibrium pH is greater than 6. The actual error in the ion balance is then divided by the final value for the equilibrium $[H^+]$ to produce the subroutine output variable ERRH. The variable HION is set equal to this final value of the equilibrium $[H^+]$ and a return to subroutine GEN is executed.

3.7.3 Subroutine DIFLIM03

DIFLIM03 is a function subprogram based on the work of Schwartz and Freiberg (1981). This subprogram returns a value for the liquid diffusion rate limiting term in the aqueous-phase O_3 - SO_2 reaction. In brief, the limited solubility of ozone can lead to situations where the concentration of ozone in the interior of a droplet is less than the equilibrium value existing at the droplet surface. The occurrence of such situations is dependent on the size of the droplet, which affects the diffusional transport time, and on the pH-dependent rate of the O_3 - SO_2 reaction, which affects how quickly the incoming ozone "disappears." When cloud droplets are large or at high pH conditions (where the O_3 - SO_2 reaction rate increases substantially), an aqueous-phase ozone concentration gradient may exist that makes the average ozone concentration within the drop less than its equilibrium value. This reduced-average ozone concentration also reduces the overall O_3 - SO_2 reaction rate within the droplet. The "effective" reaction rate can be estimated by assuming that the rate reduction is equal to the ratio of the average ozone concentration in the droplet to its equilibrium value. Schwartz and Freiberg (1981) have estimated this ratio as

$$DIFLIM03 = 3(\coth q - 1/q)/q \quad (30)$$

$$q = \left(\frac{r^2 \times k_{eff}}{D} \right)^{0.5} \quad (31)$$

where r is the droplet radius, k_{eff} is the effective first-order reaction rate of ozone and $S(IV)$, and D is the diffusivity of ozone in water. The quantity $(r^2 D^{-1})$ is the characteristic mixing time for the aqueous phase. In MCCP PLUVIUS, this characteristic mixing time (TAUMIX) is approximated by assuming a monodisperse droplet distribution with 300 cloud droplets cm^{-3} space and an ozone diffusivity of $1.2 \times 10^{-5} cm^2 s^{-1}$, thus yielding the expression

$$TAUMIX = 4.9 \times 10^3 \times CLOUD^{2/3} \quad (32)$$

where CLOUD is the liquid water content in moles of $H_2O cm^{-3}$ space. TAUMIX and k_{eff} are calculated in subroutine GEN and passed as inputs to subprogram DIFLIM03. Within the subprogram, Equation (30) is numerically approximated

by using simple empirical curve fits as described in Schwartz and Freiberg (1981).

3.8 MODEL OUTPUT

Model output can occur in two forms, depending on the application desired by the user. In this example, ASCII output is written to a file that is assigned to output unit 25 at intervals of 288 s of simulation time. This output is written by the Class II subroutine PRINT and consists of listings of vertical concentrations of each species, along with vertical temperature and pressure profiles for each output time step. The elevation of the grid is given along with the concentrations and temperatures. An output binary disk file is written every 30 s to logical unit 8 from the Class II subroutine COLLECT. Most of the information contained in the ASCII file is also in the disk file, but the latter provides a more efficient form for storage and post-processing.

ASCII model output for selected time steps are reproduced in Appendix C. This output was generated by MCCP PLUVIUS using input conditions from Section 3.4 on a Digital Equipment Corporation microVAX. Output produced by other computer systems may differ slightly because of differences in the number of significant figures held in interim calculations or similar system-dependent characteristics.

4.0 FUTURE WORK: SUGGESTED AREAS FOR MCCP PLUVIUS ENHANCEMENT

The MCCP version of PLUVIUS, like PLUVIUS MOD 5.0, focuses primarily on chemical transformations and deposition. It is a kinematic model, and the flow field must be specified outside of the main code. The present version includes only rudimentary meteorology. The orographic cloud is generated by simple adiabatic ascent of air up a specified mountain barrier using a simply specified approach flow field. Chemical transformations in the model occur in the bulk condensate, with no resolution of the cloud droplet size distribution. Other investigators have developed more sophisticated meteorological and microphysical parameterizations for use with nonprecipitating clouds of this type. A great deal of the observational and modeling work on this topic has been accomplished in the last 6 or 7 years in connection with studies conducted on England's Great Dun Fell (Baker et al. 1980; Blyth et al. 1980; Carruthers and Choularton 1982; Baker et al. 1982; Baker and Latham 1982; Carruthers and Choularton 1986; Choularton et al. 1986; and Hill et al. 1986). As further MCCP observational data are obtained and processed and MCCP model simulations are performed, we should be able to determine the meteorological detail needed in the MCCP PLUVIUS Model to make more accurate simulations of orographic cloud events. From findings of previously published studies and from PLUVIUS model applications to date, we can make several initial recommendations for the further development of the modeling approach.

Before listing the recommendations, however, we should be careful to state that the input requirements of the present model, in a number of respects, are already beyond the measurement capabilities of the existing MCCP field programs at many of the field sites. Adding further complexity to the MCCP PLUVIUS model will, no doubt, increase the input requirements of the model and require further and more extensive field studies to fully evaluate model performance. For this reason, we feel that careful consideration should be given to the role of the modeling work in the MCCP program. To the extent possible, the modeling work should be focused on gaining a better understanding of the relevant physics leading to forest dieback so that it can guide and complement the MCCP observational program. A strong interaction between the modeling and observational programs will be essential to evaluate the utility

of the model in fulfilling this role. The following are several recommendations for further development of MCCP PLUVIUS:

- **Cloud Microphysics.** Aqueous-phase chemical reactions in the present version of MCCP PLUVIUS take place in the bulk liquid cloud water. In nature, an orographic cloud contains a distribution of cloud droplet sizes. These droplets contain different concentrations of reactants depending on droplet size, the composition of the nucleus on which the droplet formed, and other characteristics of the droplet and its environment. Because reaction rates are dependent on the initial concentrations of the reactants and the overall solution acidity, we can expect different rates of reaction in droplets of different size. Thus, it seems appropriate to further develop the capability of MCCP PLUVIUS to handle detailed cloud microphysics. The new model structure, once developed, would form the basis by which entrainment could be properly simulated in the model.
- **Entrainment.** Liquid water contents in the orographic cloud are presently calculated adiabatically in the MCCP PLUVIUS Model. These calculated liquid water contents represent an upper limit to the liquid water content of a cloud. In an actual cloud, turbulent entrainment of ambient air at the cloud boundaries incorporates dry air and fresh cloud condensation nuclei into the cloud. Some of the water droplets in the cloud evaporate into the entrained dry air so that the cloud liquid water content falls below the adiabatic value. Similarly, detrainment of cloud droplets to the ambient environment at the cloud's edges results in drying of the cloud. If MCCP observations show liquid water contents below adiabatic values, this suggests that such entrainment processes are occurring in the orographic clouds studied. The sub-adiabatic liquid water contents cause modeled chemical reactions in the cloud to be simulated in solutions that are too dilute. Thus, it seems appropriate to modify the model, with the aid of observational data, to adequately account for entrainment. One can envision a hierarchy of different parameterizations of entrainment for such a cloud model. The present version of MCCP PLUVIUS includes a simple entrainment option that can account for turbulent transport across the cloud top boundary. Actual entrainment

effects in orographic clouds are more complicated, although progress in understanding and modeling these effects has been made in recent years in studies of orographic clouds at the Great Dun Fell, England (Baker et al. 1980; Blyth et al. 1980; Baker and Latham 1982; Choularton et al. 1986). The proper level of detail required to adequately model the effects of entrainment on the chemical simulations could be estimated by a careful look at MCCP field data. It would be essential to have good estimates of cloud base and top heights for these calculations.

- Two- and Three-Dimensional Simulations. The present MCCP version of PLUVIUS allows simple one-dimensional and steady-state, two-dimensional simulations of orographic clouds. Extension of the model to full two- and three-dimensional simulations could be accomplished using a new version of PLUVIUS now being completed under a DOE-supported program at Pacific Northwest Laboratory. Determination of the flow fields at the MCCP field sites would be necessary to properly support the exercise of future two- and three-dimensional versions of the code. Currently, this extensive data need is considered to be a major stumbling block, since meteorological data of this resolution are unavailable.
- Addition of Rain and Snow Species. The capability for modeling rain and snow species can be added to a future version of MCCP PLUVIUS. Because the major use of MCCP PLUVIUS will be to study cloud events, the rain and snow species were moved out of the main body of the code into subroutines to simplify interpretation of the processes modeled by MCCP PLUVIUS. Parameterization of the rain and snow species can be accomplished with little difficulty by reincorporating these processes into the code from earlier versions of MCCP PLUVIUS if this should prove desirable.
- Improved Aerosol-Gas Partitioning of Nitrogen Species. In Subroutine SETUP there is a factor that automatically partitions the total NH_4^+ and NO_3^- into the gas and particle phases according to the constant values of the AEROFACNH4 and AEROFACNO3 variables. Consideration of the equilibrium aerosol/gas/aqueous phases that exist in the $\text{NH}_4^+/\text{SO}_4^{2-}/\text{NO}_3^-$ system implies that this partitioning is not a constant value, but is, in fact, dependent on a number of other variables in the system. A subroutine

that describes the possible scenarios that may occur in this system, and partitions the phases accordingly, would be a useful addition to the MCCP PLUVIUS model, since nitrogen species may play an important role in forest dieback.

- Improved Empirical Formulation for Cloud Water Hydrogen ion Concentration. As mentioned in the discussion of the Class III subroutine HIONCALC, the MCCP PLUVIUS model can calculate the hydrogen ion concentration either through an iterative process or through an empirical formulation. The empirical expression should be based on an analysis of actual concentration data from many different precipitation measurements. The current empirical formula in MCCP PLUVIUS is based on rainwater concentrations, but the model would be improved if the empirical formulation were based on actual, site-specific cloud water measurements. Ideally, separate relationships for each season would be included. To derive such equations, the user would need to have an extensive data set of pH versus major pollutant species concentrations over many different cloud events. These data could be statistically analyzed to find the best fit expression relating hydrogen ion concentration to other major cloud water components.
- Automated Calculation of Critical Dividing Streamline Height. Dividing streamline height calculations could be automated in a special subroutine that uses rawinsonde data as input. This subroutine should be capable of running in a stand-alone interactive mode where the user inputs sounding and topographic data.
- Eddy Diffusivity. An automated procedure for estimating eddy diffusivity should be developed based on atmospheric stability, windspeed, surface roughness, or other appropriate parameters.
- Deposition Velocity. An improved treatment of cloud water deposition velocity should be developed taking into account surface vegetative cover and the presence of warm versus supercooled cloud droplets.
- Enhanced Chemistry. Additional chemical reactions could be incorporated into the model to determine the significance of these reactions for orographic cloud events. Free radical chemistry in the aqueous phase reactions and nighttime gas-phase N_2O_5 chemistry are two candidates.

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APPENDIX A

LISTINGS OF MCCP PLUVIUS CLASS I SUBROUTINES

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LISTINGS OF MCCP PLUVIUS CLASS I SUBROUTINES

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C-----
C      SUBROUTINE SETUP
C
C      THIS IS THE MCCP PLUVIUS VERSION OF SETUP
C      WHICH READS INPUT DATA FROM THE LOGICAL UNIT SPECIFIED
C      AS THE INPUT FILE.
C      THIS VERSION HANDLES ONLY GAS/CLOUD/AEROSOL SPECIES - BUT
C      LATER VERSIONS WILL HANDLE RAIN AND SNOW SPECIES (THESE
C      ARE REFLECTED IN THE PRELIMINARY PLACEMENT OF CALLS TO
C      SUBROUTINES RAIN AND SNOW; WHICH ONLY EXIST AS DO-NOTHING
C      SUBROUTINES IN THIS VERSION)
C
C      WILL RUN WITH ONLY WATER SPECIES IF NCOMP = 2
C
C      INCLUDE 'PLUVCMN'
C
C      ESTABLISH SPECIES GROUND LEVEL CONCENTRATIONS - READ FROM
C      THE INPUT FILE IN UNITS OF PPB
C
C      IF (NCOMP .LT. 3) GO TO 300
C      READ(LUNIN,*) CG_SO2,CG_SO4,CG_NO3G,CG_NO3A
C      READ(LUNIN,*) CG_NH4G, CG_NH4A, CG_CAT2
C      READ(LUNIN,*) CG_O3, CG_H2O2, CG_FORM
C      READ(LUNIN,*) RCAT1_CAT2, RAN1_CAT2, RAN2_CAT2
C
C      DEFINE VALUE FOR IWSPEC, WHERE IWSPEC IS A CONTROL
C      VARIABLE TO SPECIFY INCLUSION OF RAIN AND SNOW SPECIES.
C      IN THIS VERSION, IWSPEC IS ALWAYS 1.
C
300      CONTINUE
C      IWSPEC = 1
C
C      READ IN SURFACE WIND SPEED FROM INPUT FILE, IN CM/SEC
C
C      READ(LUNIN,700) UA
700      FORMAT(F5.1)
C
C      ESTABLISH SPECIES LOCATION VARIABLE VALUES IN SAME ORDER
C      AS IN INPUT FILE
C
C      DATA KTEMP, KVPCL, KCLD/1,2, 14/
C      DATA KSO2GC,KSO2G, KSO2C/ 3, 17, 18/

```



```

DATA KSO4A1, KSO4C/4,5/
DATA KNO3A1GC, KNO3A1, KNO3G, KNO3C / 6,23,21,22/
DATA KNH4A1GC, KNH4A1, KNH4G, KNH4C / 7, 26,24,25/
DATA KH2O2GC, KH2O2G, KH2O2C/ 8, 19, 20/
DATA KO3G/ 9/
DATA KEXCAT2, KEXCAT1 / 10, 15/
DATA KHIONC / 16/
DATA KHMSXAl, KHMSXC / 12, 13/
DATA KFORMGC,KFORMG,KFORMC / 11, 27, 28/
DATA KEXAN1, KEXAN2 / 29, 30/

C
C ESTABLISH DIFFERENT LOCATION VARIABLES IF RAIN OR SNOW
C SPECIES ARE INCLUDED

      IF (IWSPEC .EQ. 2) CALL RAIN(1)
      IF (IWSPEC .EQ. 3) CALL SNOW(1)

C
C ESTABLISH PARAMETERS USED IN O.D.E. INTEGRATION ROUTINE
C (ODEINT)
C
      DATA EPS / .05 /
      DATA DIMIN / 1.E-10 /
      DATA RATESE / 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, THEN

```

```

C   ESTABLISH WATER VAPOR PROFILE - BASED ON RELATIVE
C   HUMIDITY CALCULATED FROM THE DEWPOINT
C
      C(1,KTEMP) = TEMP0
      DO I = 1, N
        IF (Z(I) .LE. 1.75E4) THEN
          C(I,KTEMP) = -4.0E-5*Z(I) + TEMP0
        ELSE IF (Z(I) .LE. 2.75E4) THEN
          C(I,KTEMP) = 5.0E-5*(Z(I)-2.75E4) + 283.95
        ELSE
          C(I,KTEMP) = -4.0E-5*(Z(I) - 4.0E4) + 283.45
        ENDIF

        IF (Z(I) .LT. 1.0E4) THEN
          TDP = -8.0E-5*Z(I) + 283.45
        ELSE
          TDP = -1.86E-4*(Z(I)-1.0E4) + 282.65
        ENDIF

C   CONVERT INTO RELATIVE HUMIDITY
C
      RH = 10,**(2353*(1/C(I,KTEMP) - 1/TDP))
      C(I,KVAPCL) = RH*SAT( C(I,KTEMP) )
      END DO
      CALL PRESSF( 1 )

C
      IF (NCOMP .LT. 3) THEN
        KLOUD = 3
        GO TO 310
      ENDIF

C   DEFINE AEROFAC - THE FRACTION OF NUCLEATING SPECIES THAT
C   IS AEROSOL
C
      IF (CG_NO3A.GT.0.) THEN
        AEROFACNO3 = CG_NO3A / (CG_NO3A + CG_NO3G)
      ELSE
        AEROFACNO3 = 1.0E-5
      END IF
      IF (CG_NH4A.GT.0.) THEN
        AEROFACNH4 = CG_NH4A / (CG_NH4A + CG_NH4G)
      ELSE
        AEROFACNH4 = 1.0E-5
      END IF

C   ESTABLISH INITIAL CONCENTRATIONS OF OTHER SPECIES.
C
      DO 310 I = 1, N

```

```

ONEPPB = 1.0E-9*CS(I)
ZKM = 1.E-5*Z(I)
FACTOR= 1.-(ZKM/3.6)
FACTOR2 = 1.-(ZKM/4.2)
C(I,KSO2GC) = ONEPPB*FACTOR*CG_SO2
C(I,KSO4A1) = ONEPPB*FACTOR2*CG_SO4
C(I,KNO3A1GC) = ONEPPB*FACTOR*(CG_NO3G + CG_NO3A)
C(I,KNH4A1GC) = ONEPPB*FACTOR*(CG_NH4G + CG_NH4A)
C(I,KFORMGC) = ONEPPB*FACTOR*CG_FORM
C(I,KEXCAT2) = CG_CAT2*ONEPPB
C(I,KO3G) = ONEPPB*CG_O3
C(I,KH2O2GC) = ONEPPB*CG_H2O2*EXP(-ZKM/7.0)
C(I,KSO2G) = C(I,KSO2GC)
C(I,KH2O2G) = C(I,KH2O2GC)
C(I,KFORMG) = C(I,KFORMGC)
C(I,KNO3A1) = AEROFACNO3 * C(I,KNO3A1GC)
C(I,KNO3G) = C(I,KNO3A1GC) - C(I,KNO3A1)
C(I,KNH4A1) = AEROFACNH4 * C(I,KNH4A1GC)
C(I,KNH4G) = C(I,KNH4A1GC) - C(I,KNH4A1)
C(I,KEXCAT1) = RCAT1_CAT2*C(I,KEXCAT2)
C(I,KEXAN1) = RAN1_CAT2*C(I,KEXCAT2)
C(I,KEXAN2) = RAN2_CAT2*C(I,KEXCAT2)
310 CONTINUE
RETURN
END

```

```

C-----
      SUBROUTINE ADJUST

      INCLUDE 'PLUVCMN'
      DO 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
      END DO
C
      IF (IWSPEC .EQ. 3) CALL SNOW(2)
C
      RETURN
      END

```

```

C-----
      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
C
C   CALCULATE DEPOSITION VELOCITY FOR CLOUD DROPLET DEPOSITION
C   BASED ON THE PARAMETERIZATION OF LOVETT AND REINERS (1982)
C   AS A FUNCTION OF THE WIND SPEED
C
      IF (INIT .EQ. 1) THEN
         XVDB = 7.63E-2*UA - 1.25
      ENDIF
C
C   COMPUTE BOUNDARY CONDITIONS ONLY IF CLOUD IS PRESENT
C
      IF (C(1,KCLOUD) .LT. CMIN(KCLOUD)) GO TO 320
C
      FB(VAPCL) = -XVDB * C(1,KCLOUD)
C
      IF (NCOMP .LT. 3) GO TO 320
C
      FB(KSO4C) = -XVDB * C(1,KSO4C)
      FB(KSO2GC) = -XVDB * C(1,KSO2C)
      FB(KH2O2GC) = -XVDB * C(1,KH2O2C)
      FB(KNO3AlGC) = -XVDB * C(1,KNO3C)
      FB(KNH4AlGC) = -XVDB * C(1,KNH4C)
      FB(KEXCAT2) = -XVDB * C(1,KEXCAT2)
      FB(KFORMGC) = -XVDB * C(1,KFORMC)
      FB(KHMSXC) = -XVDB * C(1,KHMSXC)
320  CONTINUE
      RETURN
      END

```



```

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

      DO I = 1,N
         D(I,1) = 1.E5
         D(I,2) = 1.E5
      END DO
      IF (IWSPEC .EQ. 2) CALL RAIN(3)
      IF (IWSPEC .EQ. 3) CALL SNOW(3)
      RETURN
      END

```

```
C-----
      SUBROUTINE GRDSET
      INCLUDE 'PLUVCMN'
C
C  IN THIS EXAMPLE, USE A UNIFORM VERTICAL GRID SPACING
      Z(1) = 0.
      DO I= 2,N
          Z(I) = Z(I-1) + DZ
      END DO
      RETURN
      END
```

```

C-----
C      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 (FOR A FIRST
C      APPROXIMATION, ASSUME THAT THE SETTLING OF CLOUD
C      DROPLETS IS NEGLIGIBLE COMPARED TO DEPOSITION BY
C      IMPACTION)
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      RETURN
C      END

```

```

C-----
      SUBROUTINE TIMESP
C
C   TIMESP SETS ADVECTION-DIFFUSION INTEGRATION TIME STEP
C   THIS VERSION MAINTAINS THE COURANT NUMBER (W*DTEFF/DZ) AT
C   OR BELOW THE VALUE "COURMX", AND THE TIME STEP BELOW
C   DTMX
C   (DTEFF = EFFECTIVE TIME STEP = DT*URATIO)
C
      INCLUDE 'PLUVCMN'
      DATA COURMX, DTMX /.9, 5./

      DNEW = 1.E10
      DO 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 )
      END DO
      DT = AMIN1(DNEW*COURMX,DTMX)

      RETURN
      END

```

```

C-----
      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)
C   AND IREF IS A SPECIFIED REFERENCE LEVEL (FIXED FOR
C   THE MODEL RUN)
C   FOR ONE-DIMENSIONAL TIME-DEPENDENT SIMULATIONS WITH NO
C   SHEAR, SET URATIO(I) = 1. FOR ALL I.
C
      INCLUDE 'PLUVCMN'
C
C   FOR THIS EXAMPLE, WIND IS CONSTANT AT 750 CM/SEC
C
      DO I = 1,N
          URATIO(I) = 1
      END DO
      RETURN
      END

```

```

C-----
      SUBROUTINE VERT
      INCLUDE 'PLUVCMN'

      PARAMETER (PI = 3.1415927)

C
C   PARAMETERS DEFINING THE HYPOTHETICAL GROUND PROFILE:
C   DZGDT IS RATE OF CHANGE OF GROUND HEIGHT (ZG) WITH TIME
C
C   FOR THIS EXAMPLE USE THE MODIFIED GAUSSIAN MOUNTAIN WITH
C   A BASE 450 M FROM THE MOUNTAIN TOP. THE ACTUAL FORM OF THE
C   EQUATION DEPENDS ON THE WIND SPEED
C
C   GAUSSIAN MOUNTAIN EQN IS OF THE FORM:
C
C           
$$Z(Y) = CMULT * EXP(KEXP * (Y - LHALF) ** 2)$$

C
C   WHERE CMULT, KEXP, AND LHALF DEPEND ON THE WIND SPEED
C
C
      XLHALF = 6.15E5
      XKEXP = -2.22E-11
      CMULT = 4.5E4
      YTRAN = UA*TCLOCK - XLHALF
      DZGDT = 2.*CMULT*XKEXP*UA*(YTRAN)*EXP(XKEXP*(YTRAN**2))
      WAGRID1 = DZGDT/URATIO(1)

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

      RETURN
      END

```



```

C-----
C      SUBROUTINE GEN ( I, IGCALC, TGEN, DTAU, JPASSO )
C
C      I = VERTICAL GRID INDEX AT WHICH GEN/DECAY RATES ARE TO BE
C      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,
C      ...) PASS IN O.D.E. INTEGRATOR
C
C      INCLUDE 'PLUVCMN'
C      COMMON / AQUATEST1 / LOOPCO
C      COMMON/DISSCON/ DKW, DK0SO2, DK1SO2, DK2SO2, DK0LSO2,
C      2 DK0L2SO2,DK0HNO3, DK0NH4, DK0FORM, DK0O3, DK0H22,
C      3 FCO2AQ, FHCO3, FCO3, DK0HMSA
C
C      DATA XNC /500./
C      DATA DPS /0.3E-4/
C
C      LOOPCO = 0
C      JWRITEA = IOK
C      IOK = 1
C      KHCALC = 0
C
C      DO K = 1, NCOMP
C          GGEN(K) = 0
C          GDEC(K) = 0.
C      END DO
C
C      DEFINE LOCAL WATER AND TEMPERATURE VARIABLES
C      CALCULATE NEW CLOUD AND WATER VAPOR
C      CALCULATE WATER VAPOR SATURATION CONCENTRATIONS
C
C      TEMP = CNN(KTEMP)
C      TEMPC = TEMP-273.15
C      VSATW = SAT( TEMP )
C      VAPOR = AMIN1( CNN(KVAPCL), VSATW )
C      CLOUD = CNN(KVAPCL) - VAPOR
C      CNN(KCLOUD) = CLOUD
C
C      IF (NCOMP .LT. 3) GO TO 330
C-----
C      NO CLOUD CASE
C-----
C      IF NO CLOUD IS PRESENT SET AQUEOUS PHASE CONC TO CMIN, SET
C      GAS AND AEROSOL PHASE CONCENTRATIONS, AND RETURN
C      IF (CLOUD .LT. CMIN(KCLOUD)) THEN
C      C....HYDROGEN ION AND SULFUR SPECIES (NO HION EXCEPT IN CLOUD)

```

```

      CNN(KHIONC) = 0.0
      CNN(KSO2G) = CNN(KSO2GC)
      CNN(KSO2C) = CMIN(KSO2C)
      CNN(KSO4A1) = CNN(KSO4A1) + CNN(KSO4C)
      CNN(KSO4C) = CMIN(KSO4C)
      CNN(KH2O2G) = CNN(KH2O2GC)
      CNN(KH2O2C) = CMIN(KH2O2C)
C.....NITROGEN SPECIES
      CNN(KNO3G) = (1-AEROFACNO3)*CNN(KNO3A1GC)
      CNN(KNO3A1) = CNN(KNO3A1GC) - CNN(KNO3G)
      CNN(KNO3C) = CMIN(KNO3C)
      CNN(KNH4G) = (1-AEROFACNH4)*CNN(KNH4A1GC)
      CNN(KNH4A1) = CNN(KNH4A1GC) - CNN(KNH4G)
      CNN(KNH4C) = CMIN(KNH4C)
C.....FORMALDEHYDE
      CNN(KFORMG) = CNN(KFORMGC)
      CNN(KFORMC) = CMIN(KFORMC)
      CNN(KHMSX1) = CNN(KHMSX1) + CNN(KHMSXC)
      CNN(KHMSXC) = CMIN(KHMSXC)
      RETURN
END IF

C-----
C                      CLOUD CASE
C-----
      WATER = .018 * CLOUD          ! LITERS H2O/CC SPACE
C  COMPUTE ALL HENRY'S LAW COEFFICIENTS AND DISSOC CONSTANTS
      CALL DISSCON (TEMP, CS(I))
C  CALCULATE CONSTRAINED CATION AND ANION SPECIES
      CNN(KEXCAT1) = RCAT1_CAT2*CNN(KEXCAT2)
      CNN(KEXAN1) = RAN1_CAT2*CNN(KEXCAT2)
      CNN(KEXAN2) = RAN2_CAT2*CNN(KEXCAT2)
C  DETERMINE EQUILIBRIUM [H+] USING EITHER AN EMPIRICAL
C  RELATIONSHIP (KHCALC = 1) OR AN ION BALANCE CALCULATION.
      IF (KHCALC.EQ.1) THEN
          CNN(KHIONC) = 2.53E-7*CLOUD + 1.864*CNN(KSO4C)
          HIONX = CNN(KHIONC)/WATER    ! H+ IN MOLAR UNITS
      ELSE
          CEXCAT1W = CNN(KEXCAT1) / WATER
          CEXCAT2W = CNN(KEXCAT2) / WATER
          CEXAN1W = (CNN(KHMSXC) + CNN(KEXAN1)) / WATER
          CEXAN2W = (CNN(KSO4C) + CNN(KEXAN2)) / WATER
          CALL HIONCALC ( ERRH,
+           IOK,
+           TEMP, CS(I), WATER,
+           CEXCAT1W, CEXCAT2W, CEXAN1W, CEXAN2W,
+           HION,
+           CNN(KSO2GC),
+           CNN(KNO3A1GC),

```

```

+      CNN(KNH4ALGC)
+      )
      HIONX = HION
      CNN(KHIONC) = HIONX * WATER
END IF
C  COMPUTE GAS, AEROSOL, AQUEOUS PARTITIONING
C.....SO2
      XICSO2 = WATER*(DK0SO2 + (DK01SO2 +
+      DK012SO2/HIONX)/HIONX)
      CNN(KSO2G) = CNN(KSO2GC)/(1.+XICSO2)
      CNN(KSO2C) = CNN(KSO2GC) - CNN(KSO2G)

      CNN(KSO4C) = CNN(KSO4C) + CNN(KSO4AL)
      CNN(KSO4AL) = CMIN(KSO4AL)
C.....OXIDANTS (O3 SLIGHTLY SOLUBLE GAS;
C      CO2 + CNN(KO3G) APPROX. = CNN(KO3G))
      XICH2O2 = WATER * DK0H22
      CNN(KH2O2G) = CNN(KH2O2GC)/(1.+XICH2O2)
      CNN(KH2O2C) = CNN(KH2O2GC) - CNN(KH2O2G)
      CO2 = CNN(KO3G) * DK0O3 * WATER      !MOL/CC SPACE
C.....NITROGEN SPECIES
      XICNO3 = WATER * DK0HNO3 / HIONX
      XICNH4 = WATER * DK0NH4 * HION / DKW
      CNN(KNO3G) = CNN(KNO3ALGC)/(1.+XICNO3)
      CNN(KNO3C) = CNN(KNO3ALGC) - CNN(KNO3G)
      CNN(KNO3AL) = CMIN(KNO3AL)
      CNN(KNH4G) = CNN(KNH4ALGC)/(1.+XICNH4)
      CNN(KNH4C) = CNN(KNH4ALGC) - CNN(KNH4G)
      CNN(KNH4AL) = CMIN(KNH4AL)
C.....FORMALDEHYDE
      CNN(KFORMG) = CNN(KFORMGC)/(1.+ WATER * DK0FORM)
      CNN(KFORMC) = CNN(KFORMG) * WATER * DK0FORM
      CNN(KHMSXC) = CNN(KHMSXC) + CNN(KHMSXAL)
      CNN(KHMSXAL) = CMIN(KHMSXAL)
C
C  COMPUTE PARTITIONING OF AQUEOUS S(IV) SPECIES.  UNITS ARE
C  MOL/L H2O
      CSO2G = CNN(KSO2G)
      CSO2AQ = DK0SO2*CSO2G
      CHSO3 = DK01SO2*CSO2G/HIONX
      CSO3 = DK012SO2*CSO2G/(HIONX**2)
C
      IF (IGCALC .LE. 0) GO TO 330
      CSIV = CSO2AQ + CHSO3 + CSO3
      IF (CSIV .EQ. 0.) GO TO 330
C-----
C  REACTION RATE COEFFICIENTS AND OVERALL REACTION RATES
C-----
C  OZONE RATE COEFFICIENTS

```

```

      RK0SXOZ = 2.4E4
      RK1SXOZ = 4.245E13 * EXP(-5533.1/TEMP)
      RK2SXOZ = 7.376E16 * EXP(-5280.5/TEMP)
C   H2O2 RATE COEFFICIENTS
      RKSXH22 = 6.208E14 * EXP (-4751.2/TEMP)
      RCSXH22 = 13.0
C   S(IV) OXIDATION RATE EXPRESSIONS
C.....S(IV)-OZONE REACTION [LIQUID DIFFUSION RATE LIMITED]
      XKEFFOZ = (RK1SXOZ * CHSO3 + RK2SXOZ * CSO3)
      IF (HIONX .GE. 5.E-03) XKEFFOZ = XKEFFOZ + RK0SXOZ
2 * CSO2AQ
      TAUMIX = 4.9E3 * (CLOUD**0.667)      !CLOUDWATER
      SXOZ = XKEFFOZ * COZ * DIFLIMO3 (TAUMIX, XKEFFOZ)
C..... S(IV)-H2O2 REACTION
      SXH22 = RKSXH22 * HIONX * CHSO3 * CNN(KH2O2C)
      IF (HIONX .GE. 3.8E-03) SXH22 = SXH22 / (1. +
2      RCSXH22 * HIONX)
C.....S(IV)-CH2O REACTION (HMSA FORMATION; RATE COEFFICIENTS
C FROM BOYCE & HOFFMANN, J. PHYS. CHEM. (1984) 88:4740-4746.
      ALPHA1 = CHSO3 / CSIV
      ALPHA2 = CSO3 / CSIV
      RK1SXF = TEMP*EXP(-2.99E3/TEMP + 10.78)      !LIT H2O/MOL
      RK2SXF = TEMP*EXP(-2.46E3/TEMP + 19.95)      ! " "
      DKHFORM = 1.82E3 * EXP(-13.56 + 4041.4/TEMP)
      RKEFFSXF = (RK1SXF * ALPHA1 + RK2SXF * ALPHA2) / (1. +
2      DKHFORM)
      SXFORM = RKEFFSXF * CSIV * CNN(KFORMC)
C.....HMSA DECAY TO FORM S(IV) AND CH2O. HMSA DISSOCIATION
C CONSTANT FROM DIESTER ET AL., J. PHYS. CHEM.
      SGAINF = RKEFFSXF / DK0HMSA * CNN(KHMSXC)
C
C   COMPUTE GENERATION AND DECAY RATES FOR COMPUTED SPECIES
C
C..... SO2
      GDEC(KSO2GC) = SXH22 + SXOZ + SXFORM - SGAINF
C
C..... SO4
      GGEN(KSO4C) = SXH22 + SXOZ
C
C..... H2O2
      GDEC(KH2O2GC) = SXH22
C
C..... OZONE
      GDEC(KO3G) = SXOZ
C
C..... NO3 AND NH4: NO REACTION RATES INCLUDED IN THIS VERSION
C
C..... FORMALDEHYDE AND HMSA
      GGEN(KFORMGC) = SGAINF

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```

      GDEC(KFORMGC) = SXFORM
      GGEN(KHMSXC) = SXFORM
      GDEC(KHMSXC) = SGAINF
C
C.....INCLUDE GEN AND DEC TERMS FOR RAIN AND SNOW SPECIES
      IF (IWSPEC .LT. 2) CALL RAIN(5)
      IF (IWSPEC .EQ. 3) CALL SNOW(5)
C
330  CONTINUE
      IF (ITEMP .LE. 0) THEN
        IF (KTEMP .LE. NCOMP) THEN
          GGEN(KTEMP) = 0.
          GDEC(KTEMP) = 0.
        END IF
      END IF

      RETURN
      END

```

```

C-----
      SUBROUTINE RAIN(IPMC)
C
C   SUBROUTINE TO CALCULATE QUANTITIES RELEVANT TO RAIN
C   SPECIES WHEN IWSPEC = 2.
C *****
C   THIS IS A DO-NOTHING SUBROUTINE IN THIS VERSION OF
C   THE MCCP PLUVIUS
C *****
      RETURN
      END

C-----
      SUBROUTINE SNOW(IPMC)
C
C
C   SUBROUTINE TO CALCULATE QUANTITIES RELEVANT TO SNOW
C   SPECIES WHEN IWSPEC = 3.  SINCE RAIN WILL ALSO EXIST
C   WHEN SNOW EXISTS, THIS SUBROUTINE ALSO INCORPORATES
C   CALLS TO SUBROUTINE RAIN.
C *****
C   THIS IS A DO-NOTHING SUBROUTINE IN THIS VERSION OF
C   THE MCCP PLUVIUS
C *****
C
      RETURN
      END

```


APPENDIX B

LISTINGS OF MCCP PLUVIUS CLASS III SUBROUTINES

APPENDIX B

LISTINGS OF MCCP PLUVIUS CLASS III SUBROUTINES

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C-----
C      SUBROUTINE HIONCALC ( ERRH,
C      +      IOK,
C      +      TEMP, AIRDEN, WATER,
C      +      CEXCAT1W, CEXCAT2W, CEXAN1W, CEXAN2W,
C      +      HION,
C      +      CSO2GW,
C      +      CHNO3GW,
C      +      CNH3GW
C      +      )
C
C MAJOR SUBROUTINE PARAMETERS:
C      ERRH (OUTPUT) - CONVERGENCE PARAMETER = (ION BALANCE
C      ERROR)/HION
C      IOK (IN-OUT) - ON INPUT, VALUE OF -123 CAUSES
C      DIAGNOSTIC OUTPUT TO UNIT 42
C      ON OUTPUT, IOK=1 MEANS COMPUTATIONS WERE
C      SUCCESSFUL, OTHER VALUE MEANS ROUTINE FAILED
C      HION (IN/OUT) - HYDROGEN ION CONCENTRATION
C      (MOLE/LITER H2O)
C      ON INPUT, HOLDS AN INITIAL GUESS, FROM A PREVIOUS
C      SUBROUTINE CALL. SHOULD BE SET TO 0.0 IF NO
C      GUESS IS AVAILABLE.
C      ON OUTPUT, HOLDS CALCULATED VALUE OF H+
C
C SUBROUTINE CALCULATES HYDROGEN ION CONCENTRATION BASED ON
C CONCENTRATION OF OTHER ANIONS AND CATIONS IN SOLUTION
C (ION BALANCE APPROACH). INCLUDES PROVISION FOR OTHER
C SOLUBLE, NON-REACTIVE SPECIES VIA OF CHARGE 1 (CEXAN1W,
C CEXCAT1W) AND CHARGE 2 (CEXAN2W, CEXCAT2W). KNOWLEDGE
C OF Cl-, K+, Ca2+, Mg2+, ETC SHOULD BE LUMPED INTO THESE
C VARIABLES.
C
C ANIONS INCLUDED: HSO3-, SO3--, SO4--, NO3-, HCO3-, CO3--,
C OH-, CEXAN1W, CEXAN2W
C CATIONS INCLUDED: NH4+, CEXCAT1W, CEXCAT2W
C
C
C      COMMON/DISSCON/ DKW, DK0SO2, DK1SO2, DK2SO2, DK01SO2,
C      2 DK012SO2,DK0HNO3, DK0NH3, DK0FORM, DK0CO3, DK0H22,
C      3 FCO2AQ, FHCO3, FCO3, DK0HMSA
C

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```

COMMON / AQUATEST1 / LOOPCO
C
PARAMETER (ERRTOL = 1.E-3)
PARAMETER (LOOPMX = 100)
LOGICAL LDONE
LOOPCO = 0
JWRITEA = IOK
IOK = 1
C
C
C CALCULATE FIRST GUESS FOR HION AS FOLLOWS
C PARTITION GASES BASED ON PREVIOUS VALUE OF HION
C (PASSED IN HION)
C (AT "START-UP", VALUE IS 0 SO DEFAULT TO 2.5E-6)
C CALCULATE HION USING THIS PARTITIONING, BY SOLVING THE
C QUADRATIC EQUATION (NEGLECT DF TERM)
C ADJUST FOR DF TERM IF HION < 1.E-4
C
HIONX = HION
IF (HIONX.LE.1.E-14) HIONX = 2.5E-6
CSO2G = CSO2GW/(1.+ WATER*(DK0SO2 + (DK01SO2 +
+ DK012SO2/HIONX)/HIONX))
CHNO3G = CHNO3GW/(1. + WATER*DK0HNO3 / HIONX)
CNH3G = CNH3GW/(1.+WATER*DK0NH3 * HIONX / DKW)
AF = 1. + CNH3G*DK0NH3 / DKW
BF = (CEXCAT1W + 2.*CEXCAT2W) - (CEXAN1W + 2.*CEXAN2W)
CF = DK01SO2*CSO2G + DK0HNO3*CHNO3G + DKW + FHC03
DF = 2.*(DK012SO2*CSO2G + FCO3)
BFFF = BF/AF
CFFF = CF/AF
IF (ABS(BFFF) .LE. ABS(CFFF)) THEN
HIONX = 0.5 * (-BFFF + SQRT(BFFF * BFFF + 4.*CFFF))
ELSE
IF (ABS((4.*CFFF/BFFF)/BFFF) .GT. 1.0E-4) THEN
HIONX = 0.5 * (-BFFF + SQRT(BFFF*BFFF+4.*CFFF))
ELSE
IF (BFFF .GT. 0.0) THEN
HIONX = CFFF/BFFF
ELSE
HIONX = -BFFF
END IF
END IF
END IF
IF (HIONX .LE. 1.E-4) THEN
DO 1500 INEWTON = 1, 10
HFNC = -DF-HIONX*(CF-HIONX*(BF+HIONX*AF))
HFNC DER = -CF+HIONX*(2.*BF+HIONX*3.*AF)
HIONX = HIONX-HFNC/HFNC DER
1500 CONTINUE

```

```

      END IF
C
C   SOLVE FOR ION-BALANCE = 0, USING MODIFIED NEWTONS METHOD
C   THE ION-BALANCE IS A STRICTLY MONOTONIC FUNCTION OF HION
C
C   TWO GUESSES OF HION AND THE ASSOCIATED ION-BALANCE ARE
C   HELD (HION1, HION2, XIBAL1, XIBAL2)
C   A NEW GUESS OF HION IS FOUND BY LINEAR INTERPOLATION/
C   EXTRAPOLATION OF THE FIRST TWO VALUES
C
C   ITERATION STOPS WHEN XIBAL1 AND XIBAL2 ARE OF OPPOSITE
C   SIGN (SO THAT THE SOLUTION MUST BE BETWEEN HION1 AND
C   HION2) AND ABS(HION1-HION2) < ERRTOL*HION1
C
      LDONE = .FALSE.
2000   LOOPCO = LOOPCO + 1
C
C   CHECK FOR
C   CONVERGENCE ERROR (LOOPCO > LOOPMX)
C   LOOPCO = 1 OR 2
C   IF (LOOPCO .GT. LOOPMX) THEN
C       GOTO 3000
C   ELSE IF (LOOPCO .GT. 2) THEN
C       CONTINUE
C   ELSE IF (LOOPCO .EQ. 1) THEN
C       HION1 = HIONX
C       HION2 = HIONX
C       HION3 = HIONX
C       GOTO 2600
C   ELSE
C       (LOOPCO .EQ. 2)
C       HION1 = HION2
C       XIBAL1 = XIBAL2
C       HION3 = HION1*(1.0 - SIGN(ERRTOL,XIBAL1))
C       GOTO 2600
C   END IF
C
C   ORDER THE TWO VALUES SO ABS(XIBAL1) < ABS(XIBAL2)
C   IF (ABS(XIBAL2) .LT. ABS(XIBAL1)) THEN
C       DMY = HION1
C       HION1 = HION2
C       HION2 = DMY
C       DMY = XIBAL1
C       XIBAL1 = XIBAL2
C       XIBAL2 = DMY
C   END IF
C
C   CALCULATE NEW GUESS FOR HION (CALCULATION ORDERED THIS
C   WAY TO AVOID UNDERFLOW FROM DEL = HION3 - HION1 )

```

```

      SLOPE = (XIBAL2-XIBAL1)/(HION2-HION1)
      IF (SLOPE .NE. 0.0) THEN
        DEL = - XIBAL1/SLOPE
      ELSE
        DEL = 0.5*(HION2 - HION1 )
      END IF
      HION3 = HION1 + DEL
      DELMIN = 0.95*ERRTOL*HION1

      IF (XIBAL1) 2010, 2200, 2020
2010  IF (XIBAL2) 2400, 2200, 2300
2020  IF (XIBAL2) 2300, 2200, 2400

C   CASE OF XIBAL1 = 0.
2200  LDONE = .TRUE.
      GOTO 2600

C   CASE OF XIBAL1 AND XIBAL2 HAVE OPPOSITE SIGN
2300  IF (ABS(HION2-HION1) .LE. ERRTOL*HION1) THEN
      LDONE = .TRUE.
      GOTO 2600
    END IF

C   CASE OF XIBAL1 AND XIBAL2 HAVE SAME SIGN
C   REQUIRE ABS(HION3-HION1) >= DELMIN TO SPEED CONVERGENCE
2400  IF (ABS(DEL) .LT. DELMIN)
      +   HION3 = HION1 + SIGN( DELMIN, DEL )

2600  CONTINUE
C   MAINTAIN POSITIVE VALUE
      IF (HION3 .LE. 0.0)
      +   HION3 = AMAX1( 1.E-20, 0.1*AMIN1( HION1, HION2 ) )

      HIONX = HION3
      CSO2G = CSO2GW/(1.+ WATER*(DK0SO2 + (DK01SO2 +
      +   DK012SO2/HIONX)/HIONX) )
      CHNO3G = CHNO3GW/(1. + WATER*DK0HNO3 / HIONX)
      CNH3G = CNH3GW/(1.+WATER*DK0NH3 * HIONX / DKW)

      AF = 1. + CNH3G*DK0NH3 / DKW
      BF = (CEXCAT1W + 2.*CEXCAT2W) - (CEXAN1W + 2.*CEXAN2W)
      CF = DK01SO2*CSO2G + DK0HNO3*CHNO3G + DKW + FHCO3
      DF = 2.*(DK012SO2*CSO2G + FCO3)
      XIBAL3 = AF*HIONX + BF - ((CF + DF/HIONX)/HIONX)
      IF (JWRITEA .EQ. -123) THEN
        WRITE(42,9420) LOOPCO, HION1, HION2, HION3,
      +   XIBAL1, XIBAL2, XIBAL3
      END IF
9420  FORMAT( I4, 3(1PE14.6), 3X, 3(1PE14.6) )

```

```

        IF ( LDONE ) GOTO 3100

        HION2 = HION3
        XIBAL2 = XIBAL3
        GOTO 2000

C
C   NON-CONVERGENCE EXIT
C
3000    IOK = 0
C
C   NORMAL EXIT
C
3100    HION = HION3
        ERRH = XIBAL3/HION3
        RETURN
        END

```

```

C-----
C      SUBROUTINE DISSCON ( TEMP, AIRDEN )
C
C      SUBROUTINE TO CALCULATE DISSOCIATION AND HENRY'S LAW
C      CONSTANTS,
C
C      TK (INPUT) - LOCAL AIR TEMPERATURE (K)
C      AIRDEN (INPUT) - LOCAL AIR DENSITY (MOLE/CM**3)
C
C      OUTPUT VARIABLES ARE IN THE DISSCON COMMON BLOCK
C
C      HENRY'S LAW CONSTANTS (DK0xxx):  DEFINED AS
C      DK0 = [AQUEOUS]/[GAS],
C      PARAMETERIZED EXPRESSIONS DERIVED FROM DATA WITH DK0 IN
C      (MOLE/LITER)/ATM. MULTIPLIED BY R*T TO GIVE DK0 IN
C      UNITS OF (MOLE/LITER H2O)/(MOLE/CC SPACE) .
C      (EXCEPTION: NH3 PARAMETERION GIVES DIMENSIONLESS H
C      DIRECTLY. CONVERTED TO CC/L UNITS FOR CONSISTENCY.)
C      DISSOCIATION CONSTANTS (DK1xxx,DK2xxx):  DEFINED IN
C      STANDARD MANNER WITH UNITS OF MOL/LITER H2O.
C      DK1 = [H+][SINGLY-DISSOC]/[UNDISSOC]
C      DK2 = [H+][DOUBLY-DISSOC]/[SINGLY-DISSOC]
C      OTHER CONSTANTS:
C      R (UNIVERSAL GAS CONSTANT) IN (CC ATM)/MOL/K
C      CO2 (ATMOSPHERIC CO2 MIXING RATIO) 330E-6
C      DKW (DISSOCIATION CONSTANT FOR WATER) IN (MOL/LITER)**2
C      29 JAN 87 -- IN THIS VERSION OF DISSCON, DK0NH4 AND
C      DK0HNO3 ARE IN EFFECT DK01 TERMS SINCE NH3(AQ) AND
C      UNDISSOCIATED HNO3 SPECIES ARE NEGLECTED.  UNITS OF
C      THESE TERMS ARE CC SPACE MOL/L H2O/L H2O
C-----
C      COMMON/DISSCON/ DKW, DK0SO2, DK1SO2, DK2SO2, DK01SO2,
C      2 DK012SO2,DK0HNO3, DK0NH4, DK0FORM, DK0O3, DK0H22,
C      3 FCO2AQ, FCO3, FCO3, DK0HMSA
C      RTK=TEMP*82.06
C..... SO2 CONSTANTS
C      DK0SO2 = EXP(-10.25 +3121.72/TEMP)*RTK !CM3 AIR/LIT H2O
C      DK1SO2 = EXP(-10.965+1972.4/TEMP)
C      DK2SO2 = EXP(-23.14+1954.7/TEMP)
C      DK01SO2 = DK0SO2*DK1SO2
C      DK012SO2 = DK2SO2*DK01SO2
C..... HNO3 CONSTANTS (UNDISSOCIATED HNO3 NEGLECTED; ALL
C      AQUEOUS HNO3 ASSUMED TO EXIST AS H+ AND NO3-; VALID
C      FOR PH>0.8)
C      DK0HNO3 = EXP(4474.3/TEMP)*RTK
C..... WATER
C      DKW = 10**(-4.098-3245.2/TEMP + 2.2362E5/(TEMP*TEMP)
C      2      -3.984E7/(TEMP*TEMP*TEMP))

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```

C..... NH3 CONSTANTS (ALL DISSOLVED NH3 ASSUMED TO EXIST AS
C  NH4+; VALID FOR PH<7.2)
      DK0NH4 = 10.**(-1.60 + 4207.6 / TEMP) * 1000. * DKW
C..... H2O2 CONSTANT
      DK0H22 = EXP (-12.24 + 6981.6/TEMP) * RTK
C..... O3 CONSTANT
      DK0O3 = 1.402E-05 * EXP(2013.1/TEMP) * RTK
C..... FORMALDEHYDE CONSTANT
      DK0FORM = EXP(-12.71 + 6425/TEMP)*RTK !CM3 AIR/LIT H2O
C..... HMSA CONSTANT
      DK0HMSA = EXP (6573./TEMP - 6.71)
C..... CO2 CONSTANTS (CONC OF CO2 ASSUMED = 330 PPM * CS(I),
C  WHERE FHCO3/[H+] =[HCO3]; FCO3/[H+]/[H+] = CO3)
      DK0CO2 = (10.**((2385.7/TEMP+0.01526*TEMP-14.018)))*RTK
      DK1CO2 = 10.**(-3404.71/TEMP+14.8435-0.032786*TEMP)
      DK2CO2 = 10.**(-2902.39/TEMP+6.498-0.02379*TEMP)
      DK01CO2 = DK0CO2*DK1CO2
      DK012CO2 = DK01CO2*DK2CO2
      CO2G = 330.E-06 * AIRDEN
      FCO2AQ = DK0CO2*CO2G
      FHCO3 = DK01CO2*CO2G
      FCO3 = DK012CO2*CO2G
      RETURN
      END

```

```

C-----
C      FUNCTION DIFLIMO3 (TAUMIX, XKEFF)
C
C      DIFLIMO3 IS LIQUID DIFFUSION RATE LIMITING TERM FOR O3-STV
C      AQUEOUS REACTION, CALC FROM SCHWARTZ AND FREIBERG (1981)
C
C       $DIFLIMO3 = 3 * (\cosh(Q) - 1./Q) / Q$ 
C       $Q = \sqrt{TAUMIX * XKEFF}$ 
C      THE FUNCTIONAL FORM IS APPROXIMATED BY SIMPLE EMPIRICAL
C      CURVE FITS
C      TAUMIX = "MIXING" TIME FOR A DROPLET
C      FOR RAINDROPS, CONVECTIVE TRANSPORT DOMINATES AND
C       $TAUMIX = 0.01 \text{ S}$ 
C      FOR CLOUD DROPS, DIFFUSIVE TRANSPORT DOMINATES AND
C       $TAUMIX = R^2/D$  WHERE R IS THE DROP RADIUS AND
C      D IS THE DIFFUSIVITY OF OZONE IN WATER
C      XKEFF - "EFFECTIVE" FIRST ORDER LOSS RATE OF AQUEOUS O3
C
C       $Q = \sqrt{TAUMIX * XKEFF}$ 
C      IF (Q .LT. 1.) THEN
C          DIFLIMO3 = 1.0
C      ELSE IF (Q, LT. 3.) THEN
C           $DIFLIMO3 = 1.073 - 0.1335 * Q$ 
C      ELSE
C           $DIFLIMO3 = (3. - 3./Q)/Q$ 
C      END IF
C      RETURN
C      END

```

APPENDIX C

EXAMPLE OUTPUTS FROM MCCP PLUVIUS FOR SELECTED SIMULATION TIMES

APPENDIX C

EXAMPLE OUTPUTS FROM MCCP PLUVIUS FOR SELECTED SIMULATION TIMES

RUN ID: MCCP EXAMPLE RUN: BASE CASE VALUES

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 SO2-GC	FLUX	FLUX	2	0.00
4 SO4-A1	FLUX	FLUX	2	0.00
5 SO4-C	FLUX	FLUX	2	0.00
6 NO3-A1GC	FLUX	FLUX	2	0.00
7 NH4-A1GC	FLUX	FLUX	2	0.00
8 H2O2-GC	FLUX	FLUX	2	0.00
9 O3-G	FLUX	FLUX	2	0.00
10 EXCAT-A2	FLUX	FLUX	2	0.00
11 FORM-GC	FLUX	FLUX	2	0.00
12 HMSX-A1	FLUX	FLUX	2	0.00
13 HMSX-C	FLUX	FLUX	2	0.00

CONSTRAINED SPECIES

14 CLOUD
15 EXCAT-A1
16 HION-C
17 SO2-G
18 SO2-C
19 H2O2-G
20 H2O2-C
21 NO3-G
22 NO3-C
23 NO3-A1
24 NH4-G
25 NH4-C
26 NH4-A1
27 KFORM-G
28 KFORM-C
29 KEXAN-1
30 KEXAN-2

CONTROL DATA

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

TSTART	0.0	(0.00 HRS)	NPRINT	0
TSTOP	1150.0	(0.32 HRS)	DTPRIN	288.0
			DTCOLL	30.0

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

TCLOCK 0.00 (0.000 HRS)
DT 15.00

GLEVL (KM) 0.000
WAGRID(1) 0.21

Z(KM)	TEMP	VAPCL	SO2-GC	SO4-A1	SO4-C	NO3-ALGC	NH4-ALGC	H2O2-GC	O3-G	EXCAT-A2	FORM-GC
0.500	0.2831E+03	0.3002E-06	0.5788E-13	0.5921E-13	0.1000E-23	0.1158E-12	0.2026E-12	0.3129E-13	0.2353E-11	0.1344E-13	0.5788E-13
0.480	0.2831E+03	0.3082E-06	0.5838E-13	0.5966E-13	0.1000E-23	0.1168E-12	0.2043E-12	0.3145E-13	0.2358E-11	0.1347E-13	0.5838E-13
0.460	0.2832E+03	0.3164E-06	0.5888E-13	0.6011E-13	0.1000E-23	0.1178E-12	0.2061E-12	0.3160E-13	0.2363E-11	0.1350E-13	0.5888E-13
0.440	0.2833E+03	0.3248E-06	0.5938E-13	0.6056E-13	0.1000E-23	0.1188E-12	0.2078E-12	0.3176E-13	0.2368E-11	0.1353E-13	0.5938E-13
0.420	0.2834E+03	0.3333E-06	0.5988E-13	0.6101E-13	0.1000E-23	0.1198E-12	0.2096E-12	0.3192E-13	0.2373E-11	0.1356E-13	0.5988E-13
0.400	0.2835E+03	0.3421E-06	0.6039E-13	0.6146E-13	0.1000E-23	0.1208E-12	0.2114E-12	0.3208E-13	0.2378E-11	0.1359E-13	0.6039E-13
0.380	0.2835E+03	0.3511E-06	0.6089E-13	0.6192E-13	0.1000E-23	0.1218E-12	0.2131E-12	0.3224E-13	0.2383E-11	0.1362E-13	0.6089E-13
0.360	0.2836E+03	0.3602E-06	0.6140E-13	0.6238E-13	0.1000E-23	0.1228E-12	0.2149E-12	0.3240E-13	0.2388E-11	0.1364E-13	0.6140E-13
0.340	0.2837E+03	0.3696E-06	0.6191E-13	0.6283E-13	0.1000E-23	0.1238E-12	0.2167E-12	0.3256E-13	0.2393E-11	0.1367E-13	0.6191E-13
0.320	0.2838E+03	0.3792E-06	0.6242E-13	0.6329E-13	0.1000E-23	0.1248E-12	0.2185E-12	0.3273E-13	0.2398E-11	0.1370E-13	0.6242E-13
0.300	0.2839E+03	0.3891E-06	0.6294E-13	0.6376E-13	0.1000E-23	0.1259E-12	0.2203E-12	0.3289E-13	0.2403E-11	0.1373E-13	0.6294E-13
0.280	0.2839E+03	0.3991E-06	0.6345E-13	0.6422E-13	0.1000E-23	0.1269E-12	0.2221E-12	0.3305E-13	0.2408E-11	0.1376E-13	0.6345E-13
0.260	0.2839E+03	0.4097E-06	0.6400E-13	0.6471E-13	0.1000E-23	0.1280E-12	0.2240E-12	0.3324E-13	0.2414E-11	0.1380E-13	0.6400E-13
0.240	0.2838E+03	0.4205E-06	0.6456E-13	0.6522E-13	0.1000E-23	0.1291E-12	0.2260E-12	0.3342E-13	0.2421E-11	0.1384E-13	0.6456E-13
0.220	0.2837E+03	0.4316E-06	0.6513E-13	0.6573E-13	0.1000E-23	0.1303E-12	0.2279E-12	0.3361E-13	0.2428E-11	0.1387E-13	0.6513E-13
0.200	0.2836E+03	0.4430E-06	0.6569E-13	0.6625E-13	0.1000E-23	0.1314E-12	0.2299E-12	0.3380E-13	0.2435E-11	0.1391E-13	0.6569E-13
0.180	0.2835E+03	0.4547E-06	0.6626E-13	0.6676E-13	0.1000E-23	0.1325E-12	0.2319E-12	0.3399E-13	0.2441E-11	0.1395E-13	0.6626E-13
0.160	0.2835E+03	0.4663E-06	0.6680E-13	0.6725E-13	0.1000E-23	0.1336E-12	0.2338E-12	0.3417E-13	0.2447E-11	0.1398E-13	0.6680E-13
0.140	0.2836E+03	0.4782E-06	0.6734E-13	0.6772E-13	0.1000E-23	0.1347E-12	0.2357E-12	0.3434E-13	0.2452E-11	0.1401E-13	0.6734E-13
0.120	0.2837E+03	0.4903E-06	0.6787E-13	0.6820E-13	0.1000E-23	0.1357E-12	0.2375E-12	0.3451E-13	0.2457E-11	0.1404E-13	0.6787E-13
0.100	0.2838E+03	0.5026E-06	0.6840E-13	0.6868E-13	0.1000E-23	0.1368E-12	0.2394E-12	0.3468E-13	0.2463E-11	0.1407E-13	0.6840E-13
0.080	0.2838E+03	0.5079E-06	0.6894E-13	0.6917E-13	0.1000E-23	0.1379E-12	0.2413E-12	0.3485E-13	0.2468E-11	0.1410E-13	0.6894E-13
0.060	0.2839E+03	0.5133E-06	0.6948E-13	0.6965E-13	0.1000E-23	0.1390E-12	0.2432E-12	0.3503E-13	0.2473E-11	0.1413E-13	0.6948E-13
0.040	0.2840E+03	0.5187E-06	0.7002E-13	0.7013E-13	0.1000E-23	0.1400E-12	0.2451E-12	0.3520E-13	0.2478E-11	0.1416E-13	0.7002E-13
0.020	0.2841E+03	0.5242E-06	0.7056E-13	0.7062E-13	0.1000E-23	0.1411E-12	0.2470E-12	0.3538E-13	0.2484E-11	0.1419E-13	0.7056E-13
0.000	0.2841E+03	0.5297E-06	0.7111E-13	0.7111E-13	0.1000E-23	0.1422E-12	0.2489E-12	0.3556E-13	0.2489E-11	0.1422E-13	0.7111E-13

TCLOCK 0.00 (0.000 HRS)
DT 15.00

GLEVL (KM) 0.000
WAGRID(1) 0.21

Z(KM)	HMSX-A1	HMSX-C	CLOUD	EXCAT-A1	HION-C	SO2-G	SO2-C	H2O2-G	H2O2-C	NO3-G	NO3-C
0.500	0.2000E-23	0.1000E-23	0.0000E+00	0.1344E-13	0.0000E+00	0.5788E-13	0.1000E-23	0.3129E-13	0.1000E-23	0.8682E-13	0.1000E-23
0.480	0.2000E-23	0.1000E-23	0.0000E+00	0.1347E-13	0.0000E+00	0.5838E-13	0.1000E-23	0.3145E-13	0.1000E-23	0.8757E-13	0.1000E-23
0.460	0.2000E-23	0.1000E-23	0.0000E+00	0.1350E-13	0.0000E+00	0.5888E-13	0.1000E-23	0.3160E-13	0.1000E-23	0.8831E-13	0.1000E-23
0.440	0.2000E-23	0.1000E-23	0.0000E+00	0.1353E-13	0.0000E+00	0.5938E-13	0.1000E-23	0.3176E-13	0.1000E-23	0.8907E-13	0.1000E-23
0.420	0.2000E-23	0.1000E-23	0.0000E+00	0.1356E-13	0.0000E+00	0.5988E-13	0.1000E-23	0.3192E-13	0.1000E-23	0.8982E-13	0.1000E-23
0.400	0.2000E-23	0.1000E-23	0.0000E+00	0.1359E-13	0.0000E+00	0.6039E-13	0.1000E-23	0.3208E-13	0.1000E-23	0.9058E-13	0.1000E-23
0.380	0.2000E-23	0.1000E-23	0.0000E+00	0.1362E-13	0.0000E+00	0.6089E-13	0.1000E-23	0.3224E-13	0.1000E-23	0.9134E-13	0.1000E-23
0.360	0.2000E-23	0.1000E-23	0.0000E+00	0.1364E-13	0.0000E+00	0.6140E-13	0.1000E-23	0.3240E-13	0.1000E-23	0.9210E-13	0.1000E-23
0.340	0.2000E-23	0.1000E-23	0.0000E+00	0.1367E-13	0.0000E+00	0.6191E-13	0.1000E-23	0.3256E-13	0.1000E-23	0.9287E-13	0.1000E-23
0.320	0.2000E-23	0.1000E-23	0.0000E+00	0.1370E-13	0.0000E+00	0.6242E-13	0.1000E-23	0.3273E-13	0.1000E-23	0.9364E-13	0.1000E-23
0.300	0.2000E-23	0.1000E-23	0.0000E+00	0.1373E-13	0.0000E+00	0.6294E-13	0.1000E-23	0.3289E-13	0.1000E-23	0.9441E-13	0.1000E-23
0.280	0.2000E-23	0.1000E-23	0.0000E+00	0.1376E-13	0.0000E+00	0.6345E-13	0.1000E-23	0.3305E-13	0.1000E-23	0.9518E-13	0.1000E-23
0.260	0.2000E-23	0.1000E-23	0.0000E+00	0.1380E-13	0.0000E+00	0.6400E-13	0.1000E-23	0.3324E-13	0.1000E-23	0.9600E-13	0.1000E-23
0.240	0.2000E-23	0.1000E-23	0.0000E+00	0.1384E-13	0.0000E+00	0.6456E-13	0.1000E-23	0.3342E-13	0.1000E-23	0.9685E-13	0.1000E-23
0.220	0.2000E-23	0.1000E-23	0.0000E+00	0.1387E-13	0.0000E+00	0.6513E-13	0.1000E-23	0.3361E-13	0.1000E-23	0.9769E-13	0.1000E-23
0.200	0.2000E-23	0.1000E-23	0.0000E+00	0.1391E-13	0.0000E+00	0.6569E-13	0.1000E-23	0.3380E-13	0.1000E-23	0.9854E-13	0.1000E-23
0.180	0.2000E-23	0.1000E-23	0.0000E+00	0.1395E-13	0.0000E+00	0.6626E-13	0.1000E-23	0.3399E-13	0.1000E-23	0.9940E-13	0.1000E-23
0.160	0.2000E-23	0.1000E-23	0.0000E+00	0.1398E-13	0.0000E+00	0.6680E-13	0.1000E-23	0.3417E-13	0.1000E-23	0.1002E-12	0.1000E-23
0.140	0.2000E-23	0.1000E-23	0.0000E+00	0.1401E-13	0.0000E+00	0.6734E-13	0.1000E-23	0.3434E-13	0.1000E-23	0.1010E-12	0.1000E-23
0.120	0.2000E-23	0.1000E-23	0.0000E+00	0.1404E-13	0.0000E+00	0.6787E-13	0.1000E-23	0.3451E-13	0.1000E-23	0.1018E-12	0.1000E-23
0.100	0.2000E-23	0.1000E-23	0.0000E+00	0.1407E-13	0.0000E+00	0.6840E-13	0.1000E-23	0.3468E-13	0.1000E-23	0.1026E-12	0.1000E-23
0.080	0.2000E-23	0.1000E-23	0.0000E+00	0.1410E-13	0.0000E+00	0.6894E-13	0.1000E-23	0.3485E-13	0.1000E-23	0.1034E-12	0.1000E-23
0.060	0.2000E-23	0.1000E-23	0.0000E+00	0.1413E-13	0.0000E+00	0.6948E-13	0.1000E-23	0.3503E-13	0.1000E-23	0.1042E-12	0.1000E-23
0.040	0.2000E-23	0.1000E-23	0.0000E+00	0.1416E-13	0.0000E+00	0.7002E-13	0.1000E-23	0.3520E-13	0.1000E-23	0.1050E-12	0.1000E-23
0.020	0.2000E-23	0.1000E-23	0.0000E+00	0.1419E-13	0.0000E+00	0.7056E-13	0.1000E-23	0.3538E-13	0.1000E-23	0.1058E-12	0.1000E-23
0.000	0.2000E-23	0.1000E-23	0.0000E+00	0.1422E-13	0.0000E+00	0.7111E-13	0.1000E-23	0.3556E-13	0.1000E-23	0.1067E-12	0.1000E-23

C,4

TCLOCK 0.00 (0.000 HRS)
DT 15.00

GLEVL (KM) 0.000
WAGRID(1) 0.21

Z(KM)	NO3-A1	NH4-G	NH4-C	NH4-A1	KFORM-G	KFORM-C	KEXAN-1	KEXAN-2	P	CS
0.500	0.2894E-13	0.5788E-13	0.1000E-23	0.1447E-12	0.5788E-13	0.1000E-23	0.1344E-13	0.1344E-13	0.7909E+06	0.3361E-04
0.480	0.2919E-13	0.5838E-13	0.1000E-23	0.1459E-12	0.5838E-13	0.1000E-23	0.1347E-13	0.1347E-13	0.7928E+06	0.3368E-04
0.460	0.2944E-13	0.5888E-13	0.1000E-23	0.1472E-12	0.5888E-13	0.1000E-23	0.1350E-13	0.1350E-13	0.7947E+06	0.3375E-04
0.440	0.2969E-13	0.5938E-13	0.1000E-23	0.1484E-12	0.5938E-13	0.1000E-23	0.1353E-13	0.1353E-13	0.7967E+06	0.3382E-04
0.420	0.2994E-13	0.5988E-13	0.1000E-23	0.1497E-12	0.5988E-13	0.1000E-23	0.1356E-13	0.1356E-13	0.7986E+06	0.3389E-04
0.400	0.3019E-13	0.6039E-13	0.1000E-23	0.1510E-12	0.6039E-13	0.1000E-23	0.1359E-13	0.1359E-13	0.8005E+06	0.3397E-04
0.380	0.3045E-13	0.6089E-13	0.1000E-23	0.1522E-12	0.6089E-13	0.1000E-23	0.1362E-13	0.1362E-13	0.8024E+06	0.3404E-04
0.360	0.3070E-13	0.6140E-13	0.1000E-23	0.1535E-12	0.6140E-13	0.1000E-23	0.1364E-13	0.1364E-13	0.8044E+06	0.3411E-04
0.340	0.3096E-13	0.6191E-13	0.1000E-23	0.1548E-12	0.6191E-13	0.1000E-23	0.1367E-13	0.1367E-13	0.8063E+06	0.3418E-04
0.320	0.3121E-13	0.6242E-13	0.1000E-23	0.1561E-12	0.6242E-13	0.1000E-23	0.1370E-13	0.1370E-13	0.8083E+06	0.3426E-04
0.300	0.3147E-13	0.6294E-13	0.1000E-23	0.1573E-12	0.6294E-13	0.1000E-23	0.1373E-13	0.1373E-13	0.8102E+06	0.3433E-04
0.280	0.3173E-13	0.6345E-13	0.1000E-23	0.1586E-12	0.6345E-13	0.1000E-23	0.1376E-13	0.1376E-13	0.8122E+06	0.3440E-04
0.260	0.3200E-13	0.6400E-13	0.1000E-23	0.1600E-12	0.6400E-13	0.1000E-23	0.1380E-13	0.1380E-13	0.8141E+06	0.3449E-04
0.240	0.3228E-13	0.6456E-13	0.1000E-23	0.1614E-12	0.6456E-13	0.1000E-23	0.1384E-13	0.1384E-13	0.8161E+06	0.3459E-04
0.220	0.3256E-13	0.6513E-13	0.1000E-23	0.1628E-12	0.6513E-13	0.1000E-23	0.1387E-13	0.1387E-13	0.8180E+06	0.3468E-04
0.200	0.3285E-13	0.6569E-13	0.1000E-23	0.1642E-12	0.6569E-13	0.1000E-23	0.1391E-13	0.1391E-13	0.8200E+06	0.3478E-04
0.180	0.3313E-13	0.6626E-13	0.1000E-23	0.1657E-12	0.6626E-13	0.1000E-23	0.1395E-13	0.1395E-13	0.8220E+06	0.3488E-04
0.160	0.3340E-13	0.6680E-13	0.1000E-23	0.1670E-12	0.6680E-13	0.1000E-23	0.1398E-13	0.1398E-13	0.8240E+06	0.3496E-04
0.140	0.3367E-13	0.6734E-13	0.1000E-23	0.1683E-12	0.6734E-13	0.1000E-23	0.1401E-13	0.1401E-13	0.8260E+06	0.3503E-04
0.120	0.3393E-13	0.6787E-13	0.1000E-23	0.1697E-12	0.6787E-13	0.1000E-23	0.1404E-13	0.1404E-13	0.8280E+06	0.3510E-04
0.100	0.3420E-13	0.6840E-13	0.1000E-23	0.1710E-12	0.6840E-13	0.1000E-23	0.1407E-13	0.1407E-13	0.8300E+06	0.3518E-04
0.080	0.3447E-13	0.6894E-13	0.1000E-23	0.1724E-12	0.6894E-13	0.1000E-23	0.1410E-13	0.1410E-13	0.8320E+06	0.3525E-04
0.060	0.3474E-13	0.6948E-13	0.1000E-23	0.1737E-12	0.6948E-13	0.1000E-23	0.1413E-13	0.1413E-13	0.8340E+06	0.3533E-04
0.040	0.3501E-13	0.7002E-13	0.1000E-23	0.1751E-12	0.7002E-13	0.1000E-23	0.1416E-13	0.1416E-13	0.8360E+06	0.3540E-04
0.020	0.3528E-13	0.7056E-13	0.1000E-23	0.1764E-12	0.7056E-13	0.1000E-23	0.1419E-13	0.1419E-13	0.8380E+06	0.3548E-04
0.000	0.3556E-13	0.7111E-13	0.1000E-23	0.1778E-12	0.7111E-13	0.1000E-23	0.1422E-13	0.1422E-13	0.8400E+06	0.3556E-04

TCLOCK 870.00 (0.242 HRS)
DT 5.00

GLEVL (KM) 0.437
WAGRID(1) -49.31

Z(KM)	TEMP	VAPCL	SO2-GC	SO4-A1	SO4-C	NO3-ALGC	NH4-ALGC	H2O2-GC	O3-G	EXCAT-A2	FORM-GC
0.937	0.2781E+03	0.3280E-06	0.5740E-13	0.5841E-13	0.1000E-23	0.1148E-12	0.2009E-12	0.3047E-13	0.2257E-11	0.1289E-13	0.5740E-13
0.917	0.2783E+03	0.3291E-06	0.5752E-13	0.5853E-13	0.1000E-23	0.1150E-12	0.2013E-12	0.3053E-13	0.2260E-11	0.1292E-13	0.5752E-13
0.897	0.2785E+03	0.3310E-06	0.5767E-13	0.5867E-13	0.1000E-23	0.1153E-12	0.2018E-12	0.3059E-13	0.2264E-11	0.1293E-13	0.5767E-13
0.877	0.2786E+03	0.3340E-06	0.5785E-13	0.5884E-13	0.1000E-23	0.1157E-12	0.2025E-12	0.3065E-13	0.2267E-11	0.1295E-13	0.5785E-13
0.857	0.2788E+03	0.3377E-06	0.5807E-13	0.5904E-13	0.1000E-23	0.1161E-12	0.2033E-12	0.3073E-13	0.2269E-11	0.1297E-13	0.5807E-13
0.837	0.2789E+03	0.3424E-06	0.5833E-13	0.5927E-13	0.1000E-23	0.1167E-12	0.2041E-12	0.3081E-13	0.2272E-11	0.1298E-13	0.5833E-13
0.817	0.2790E+03	0.3478E-06	0.5861E-13	0.5953E-13	0.1000E-23	0.1172E-12	0.2051E-12	0.3090E-13	0.2275E-11	0.1300E-13	0.5861E-13
0.797	0.2791E+03	0.3540E-06	0.5894E-13	0.5982E-13	0.1000E-23	0.1179E-12	0.2063E-12	0.3100E-13	0.2278E-11	0.1302E-13	0.5894E-13
0.777	0.2792E+03	0.3608E-06	0.5929E-13	0.6014E-13	0.1000E-23	0.1186E-12	0.2075E-12	0.3111E-13	0.2281E-11	0.1304E-13	0.5929E-13
0.757	0.2792E+03	0.3682E-06	0.5967E-13	0.6050E-13	0.1000E-23	0.1194E-12	0.2089E-12	0.3123E-13	0.2285E-11	0.1306E-13	0.5968E-13
0.737	0.2793E+03	0.3761E-06	0.6006E-13	0.6090E-13	0.1000E-23	0.1202E-12	0.2103E-12	0.3134E-13	0.2290E-11	0.1308E-13	0.6010E-13
0.717	0.2794E+03	0.3844E-06	0.6045E-13	0.6136E-13	0.1000E-23	0.1211E-12	0.2119E-12	0.3142E-13	0.2295E-11	0.1311E-13	0.6055E-13
0.697	0.2795E+03	0.3930E-06	0.6079E-13	0.6190E-13	0.1000E-23	0.1220E-12	0.2135E-12	0.3145E-13	0.2300E-11	0.1314E-13	0.6102E-13
0.677	0.2796E+03	0.4017E-06	0.6101E-13	0.6259E-13	0.1000E-23	0.1229E-12	0.2151E-12	0.3134E-13	0.2306E-11	0.1317E-13	0.6150E-13
0.657	0.2797E+03	0.4105E-06	0.6100E-13	0.6348E-13	0.1000E-23	0.1238E-12	0.2167E-12	0.3099E-13	0.2313E-11	0.1320E-13	0.6199E-13
0.637	0.2799E+03	0.4192E-06	0.6064E-13	0.6466E-13	0.1000E-23	0.1245E-12	0.2179E-12	0.3027E-13	0.2320E-11	0.1321E-13	0.6247E-13
0.617	0.2800E+03	0.4277E-06	0.5903E-13	0.1000E-23	0.6615E-13	0.1250E-12	0.2187E-12	0.2906E-13	0.2327E-11	0.1319E-13	0.6294E-13
0.597	0.2801E+03	0.4359E-06	0.5902E-13	0.1000E-23	0.6729E-13	0.1248E-12	0.2184E-12	0.2778E-13	0.2334E-11	0.1311E-13	0.6334E-13
0.577	0.2803E+03	0.4435E-06	0.5845E-13	0.1000E-23	0.6762E-13	0.1236E-12	0.2163E-12	0.2660E-13	0.2341E-11	0.1292E-13	0.6363E-13
0.557	0.2804E+03	0.4506E-06	0.5813E-13	0.1000E-23	0.6676E-13	0.1206E-12	0.2110E-12	0.2540E-13	0.2347E-11	0.1255E-13	0.6371E-13
0.537	0.2806E+03	0.4569E-06	0.5804E-13	0.1000E-23	0.6426E-13	0.1150E-12	0.2013E-12	0.2400E-13	0.2354E-11	0.1192E-13	0.6341E-13
0.517	0.2807E+03	0.4624E-06	0.5815E-13	0.1000E-23	0.5959E-13	0.1058E-12	0.1852E-12	0.2218E-13	0.2360E-11	0.1094E-13	0.6249E-13
0.497	0.2809E+03	0.4670E-06	0.5842E-13	0.1000E-23	0.5227E-13	0.9225E-13	0.1615E-12	0.1970E-13	0.2366E-11	0.9506E-14	0.6063E-13
0.477	0.2810E+03	0.4706E-06	0.5874E-13	0.1000E-23	0.4206E-13	0.7382E-13	0.1293E-12	0.1636E-13	0.2371E-11	0.7593E-14	0.5745E-13
0.457	0.2811E+03	0.4731E-06	0.5896E-13	0.1000E-23	0.2908E-13	0.5080E-13	0.8902E-13	0.1212E-13	0.2376E-11	0.5220E-14	0.5265E-13
0.437	0.2812E+03	0.4747E-06	0.5886E-13	0.1000E-23	0.1394E-13	0.2424E-13	0.4257E-13	0.7115E-14	0.2382E-11	0.2496E-14	0.4622E-13

TCLOCK 870.00 (0.242 HRS)
DT 5.00

GLEVL (KM) 0.437
WAGRID(1) -49.31

Z(KM)	HMSX-A1	HMSX-C	CLOUD	EXCAT-A1	HION-C	SO2-G	SO2-C	H2O2-G	H2O2-C	NO3-G	NO3-C
0.937	0.1179E-21	0.1000E-23	0.0000E+00	0.1344E-13	0.0000E+00	0.5740E-13	0.1000E-23	0.3047E-13	0.1000E-23	0.0611E-13	0.1000E-23
0.917	0.1101E-21	0.1000E-23	0.0000E+00	0.1347E-13	0.0000E+00	0.5752E-13	0.1000E-23	0.3053E-13	0.1000E-23	0.0628E-13	0.1000E-23
0.897	0.1183E-21	0.1000E-23	0.0000E+00	0.1350E-13	0.0000E+00	0.5767E-13	0.1000E-23	0.3059E-13	0.1000E-23	0.0651E-13	0.1000E-23
0.877	0.1186E-21	0.1000E-23	0.0000E+00	0.1353E-13	0.0000E+00	0.5785E-13	0.1000E-23	0.3065E-13	0.1000E-23	0.0678E-13	0.1000E-23
0.857	0.1196E-21	0.1000E-23	0.0000E+00	0.1356E-13	0.0000E+00	0.5807E-13	0.1000E-23	0.3073E-13	0.1000E-23	0.0711E-13	0.1000E-23
0.837	0.1232E-21	0.1000E-23	0.0000E+00	0.1359E-13	0.0000E+00	0.5833E-13	0.1000E-23	0.3081E-13	0.1000E-23	0.0749E-13	0.1000E-23
0.817	0.1359E-21	0.1000E-23	0.0000E+00	0.1362E-13	0.0000E+00	0.5861E-13	0.1000E-23	0.3090E-13	0.1000E-23	0.0792E-13	0.1000E-23
0.797	0.1792E-21	0.1000E-23	0.0000E+00	0.1364E-13	0.0000E+00	0.5894E-13	0.1000E-23	0.3100E-13	0.1000E-23	0.0841E-13	0.1000E-23
0.777	0.3204E-21	0.1000E-23	0.0000E+00	0.1367E-13	0.0000E+00	0.5929E-13	0.1000E-23	0.3111E-13	0.1000E-23	0.0894E-13	0.1000E-23
0.757	0.7577E-21	0.1000E-23	0.0000E+00	0.1370E-13	0.0000E+00	0.5967E-13	0.1000E-23	0.3123E-13	0.1000E-23	0.0952E-13	0.1000E-23
0.737	0.2044E-20	0.1000E-23	0.0000E+00	0.1373E-13	0.0000E+00	0.6006E-13	0.1000E-23	0.3134E-13	0.1000E-23	0.0915E-13	0.1000E-23
0.717	0.5615E-20	0.1000E-23	0.0000E+00	0.1376E-13	0.0000E+00	0.6045E-13	0.1000E-23	0.3142E-13	0.1000E-23	0.0908E-13	0.1000E-23
0.697	0.1494E-19	0.1000E-23	0.0000E+00	0.1380E-13	0.0000E+00	0.6079E-13	0.1000E-23	0.3145E-13	0.1000E-23	0.0915E-13	0.1000E-23
0.677	0.3769E-19	0.1000E-23	0.0000E+00	0.1384E-13	0.0000E+00	0.6101E-13	0.1000E-23	0.3134E-13	0.1000E-23	0.0922E-13	0.1000E-23
0.657	0.8930E-19	0.1000E-23	0.0000E+00	0.1387E-13	0.0000E+00	0.6100E-13	0.1000E-23	0.3099E-13	0.1000E-23	0.0928E-13	0.1000E-23
0.637	0.1974E-18	0.1000E-23	0.0000E+00	0.1322E-13	0.0000E+00	0.6064E-13	0.1000E-23	0.3027E-13	0.1000E-23	0.0934E-13	0.1000E-23
0.617	0.1000E-23	0.4042E-18	0.2054E-08	0.1319E-13	0.3874E-13	0.5983E-13	0.2487E-17	0.2276E-13	0.6301E-14	0.1771E-16	0.1250E-12
0.597	0.1000E-23	0.7502E-18	0.6579E-08	0.1311E-13	0.4119E-13	0.5900E-13	0.2269E-16	0.1460E-13	0.1298E-13	0.1846E-17	0.1248E-12
0.577	0.1000E-23	0.1256E-17	0.1005E-07	0.1292E-13	0.4200E-13	0.5840E-13	0.4975E-16	0.1145E-13	0.1515E-13	0.0198E-18	0.1236E-12
0.557	0.1000E-23	0.1909E-17	0.1277E-07	0.1255E-13	0.4334E-13	0.5805E-13	0.7797E-16	0.9553E-14	0.1585E-13	0.5057E-18	0.1206E-12
0.537	0.1000E-23	0.2684E-17	0.1483E-07	0.1192E-13	0.4255E-13	0.5794E-13	0.1057E-15	0.8273E-14	0.1573E-13	0.3542E-18	0.1150E-12
0.517	0.1000E-23	0.3546E-17	0.1620E-07	0.1094E-13	0.4009E-13	0.5802E-13	0.1328E-15	0.7266E-14	0.1491E-13	0.2592E-18	0.1058E-12
0.497	0.1000E-23	0.4421E-17	0.1687E-07	0.9506E-14	0.3566E-13	0.5826E-13	0.1611E-15	0.6327E-14	0.1337E-13	0.1867E-18	0.9225E-13
0.477	0.1000E-23	0.5105E-17	0.1679E-07	0.7593E-14	0.2906E-13	0.5855E-13	0.1951E-15	0.5312E-14	0.1105E-13	0.1237E-18	0.7382E-13
0.457	0.1000E-23	0.5120E-17	0.1594E-07	0.5220E-14	0.2040E-13	0.5871E-13	0.2494E-15	0.4101E-14	0.8023E-14	0.6668E-19	0.5080E-13
0.437	0.1000E-23	0.3365E-17	0.1432E-07	0.2496E-14	0.1017E-13	0.5846E-13	0.3988E-15	0.2595E-14	0.4520E-14	0.1978E-19	0.2424E-13

TCLOCK 870.00 (0.242 HRS)
DT 5.00

GLEVL (KM) 0.437
WAGRID(1) -49.31

Z(KM)	N03-A1	NH4-G	NH4-C	NH4-A1	RFORM-G	RFORM-C	KEXAN-1	KEXAN-2	P	CS
0.937	0.2870E-13	0.5740E-13	0.1000E-23	0.1435E-12	0.5740E-13	0.1000E-23	0.1344E-13	0.1344E-13	0.7495E+06	0.3241E-04
0.917	0.2876E-13	0.5752E-13	0.1000E-23	0.1438E-12	0.5752E-13	0.1000E-23	0.1347E-13	0.1347E-13	0.7514E+06	0.3247E-04
0.897	0.2884E-13	0.5767E-13	0.1000E-23	0.1442E-12	0.5767E-13	0.1000E-23	0.1350E-13	0.1350E-13	0.7532E+06	0.3253E-04
0.877	0.2893E-13	0.5785E-13	0.1000E-23	0.1446E-12	0.5785E-13	0.1000E-23	0.1353E-13	0.1353E-13	0.7551E+06	0.3259E-04
0.857	0.2904E-13	0.5807E-13	0.1000E-23	0.1452E-12	0.5807E-13	0.1000E-23	0.1356E-13	0.1356E-13	0.7569E+06	0.3266E-04
0.837	0.2916E-13	0.5833E-13	0.1000E-23	0.1458E-12	0.5833E-13	0.1000E-23	0.1359E-13	0.1359E-13	0.7588E+06	0.3272E-04
0.817	0.2931E-13	0.5861E-13	0.1000E-23	0.1465E-12	0.5861E-13	0.1000E-23	0.1362E-13	0.1362E-13	0.7607E+06	0.3279E-04
0.797	0.2947E-13	0.5894E-13	0.1000E-23	0.1473E-12	0.5894E-13	0.1000E-23	0.1364E-13	0.1364E-13	0.7625E+06	0.3286E-04
0.777	0.2965E-13	0.5929E-13	0.1000E-23	0.1482E-12	0.5929E-13	0.1000E-23	0.1367E-13	0.1367E-13	0.7644E+06	0.3293E-04
0.757	0.2984E-13	0.5968E-13	0.1000E-23	0.1492E-12	0.5968E-13	0.1000E-23	0.1370E-13	0.1370E-13	0.7663E+06	0.3301E-04
0.737	0.3005E-13	0.6010E-13	0.1000E-23	0.1502E-12	0.6010E-13	0.1000E-23	0.1373E-13	0.1373E-13	0.7681E+06	0.3308E-04
0.717	0.3027E-13	0.6054E-13	0.1000E-23	0.1514E-12	0.6055E-13	0.1000E-23	0.1376E-13	0.1376E-13	0.7700E+06	0.3315E-04
0.697	0.3050E-13	0.6100E-13	0.1000E-23	0.1525E-12	0.6102E-13	0.1000E-23	0.1380E-13	0.1380E-13	0.7719E+06	0.3322E-04
0.677	0.3073E-13	0.6146E-13	0.1000E-23	0.1537E-12	0.6150E-13	0.1000E-23	0.1384E-13	0.1384E-13	0.7738E+06	0.3329E-04
0.657	0.3095E-13	0.6190E-13	0.1000E-23	0.1548E-12	0.6199E-13	0.1000E-23	0.1387E-13	0.1387E-13	0.7757E+06	0.3335E-04
0.637	0.3114E-13	0.6227E-13	0.1000E-23	0.1557E-12	0.6247E-13	0.1000E-23	0.1322E-13	0.1322E-13	0.7776E+06	0.3341E-04
0.617	0.1000E-23	0.2110E-15	0.2185E-12	0.1000E-23	0.6140E-13	0.1457E-14	0.1319E-13	0.1319E-13	0.7795E+06	0.3348E-04
0.597	0.1000E-23	0.2014E-15	0.2182E-12	0.1000E-23	0.5892E-13	0.4427E-14	0.1311E-13	0.1311E-13	0.7814E+06	0.3355E-04
0.577	0.1000E-23	0.1954E-15	0.2161E-12	0.1000E-23	0.5715E-13	0.6484E-14	0.1292E-13	0.1292E-13	0.7833E+06	0.3361E-04
0.557	0.1000E-23	0.1919E-15	0.2100E-12	0.1000E-23	0.5576E-13	0.7945E-14	0.1255E-13	0.1255E-13	0.7852E+06	0.3368E-04
0.537	0.1000E-23	0.1899E-15	0.2011E-12	0.1000E-23	0.5450E-13	0.8909E-14	0.1192E-13	0.1192E-13	0.7871E+06	0.3374E-04
0.517	0.1000E-23	0.1888E-15	0.1851E-12	0.1000E-23	0.5311E-13	0.9382E-14	0.1094E-13	0.1094E-13	0.7890E+06	0.3381E-04
0.497	0.1000E-23	0.1881E-15	0.1613E-12	0.1000E-23	0.5130E-13	0.9336E-14	0.9506E-14	0.9506E-14	0.7910E+06	0.3387E-04
0.477	0.1000E-23	0.1876E-15	0.1291E-12	0.1000E-23	0.4871E-13	0.8739E-14	0.7593E-14	0.7593E-14	0.7929E+06	0.3394E-04
0.457	0.1000E-23	0.1866E-15	0.8884E-13	0.1000E-23	0.4504E-13	0.7604E-14	0.5220E-14	0.5220E-14	0.7948E+06	0.3401E-04
0.437	0.1000E-23	0.1808E-15	0.4239E-13	0.1000E-23	0.4018E-13	0.6042E-14	0.2496E-14	0.2496E-14	0.7967E+06	0.3408E-04

TCLOCK 1150.00 (0.319 HRS)
DT 5.00

GLEVL (KM) 0.118
WAGRID(1) -97.67

Z(KM)	TEMP	VAPCL	SO2-GC	SO4-AI	SO4-C	NO3-AIGC	NH4-AIGC	H2O2-GC	O3-G	EXCAT-A2	FORM-GC
0.618	0.2811E+03	0.3442E-06	0.5935E-13	0.6035E-13	0.1000E-23	0.1187E-12	0.2077E-12	0.3142E-13	0.2321E-11	0.1327E-13	0.5935E-13
0.598	0.2813E+03	0.3453E-06	0.5948E-13	0.6048E-13	0.1000E-23	0.1190E-12	0.2082E-12	0.3148E-13	0.2326E-11	0.1329E-13	0.5948E-13
0.578	0.2815E+03	0.3474E-06	0.5966E-13	0.6066E-13	0.1000E-23	0.1193E-12	0.2088E-12	0.3156E-13	0.2331E-11	0.1332E-13	0.5966E-13
0.558	0.2817E+03	0.3504E-06	0.5988E-13	0.6087E-13	0.1000E-23	0.1198E-12	0.2096E-12	0.3164E-13	0.2336E-11	0.1335E-13	0.5989E-13
0.538	0.2818E+03	0.3542E-06	0.6013E-13	0.6113E-13	0.1000E-23	0.1203E-12	0.2105E-12	0.3174E-13	0.2341E-11	0.1338E-13	0.6015E-13
0.518	0.2819E+03	0.3589E-06	0.6041E-13	0.6142E-13	0.1000E-23	0.1209E-12	0.2115E-12	0.3183E-13	0.2346E-11	0.1340E-13	0.6045E-13
0.498	0.2820E+03	0.3642E-06	0.6070E-13	0.6175E-13	0.1000E-23	0.1215E-12	0.2127E-12	0.3191E-13	0.2351E-11	0.1343E-13	0.6077E-13
0.478	0.2821E+03	0.3702E-06	0.6099E-13	0.6211E-13	0.1000E-23	0.1222E-12	0.2138E-12	0.3197E-13	0.2356E-11	0.1346E-13	0.6112E-13
0.458	0.2823E+03	0.3768E-06	0.6128E-13	0.6252E-13	0.1000E-23	0.1229E-12	0.2151E-12	0.3200E-13	0.2361E-11	0.1348E-13	0.6149E-13
0.438	0.2824E+03	0.3839E-06	0.6153E-13	0.6297E-13	0.1000E-23	0.1236E-12	0.2163E-12	0.3197E-13	0.2366E-11	0.1350E-13	0.6188E-13
0.418	0.2824E+03	0.3914E-06	0.6172E-13	0.6348E-13	0.1000E-23	0.1243E-12	0.2174E-12	0.3187E-13	0.2371E-11	0.1351E-13	0.6227E-13
0.398	0.2825E+03	0.3992E-06	0.6185E-13	0.6402E-13	0.1000E-23	0.1248E-12	0.2184E-12	0.3166E-13	0.2376E-11	0.1351E-13	0.6267E-13
0.378	0.2826E+03	0.4072E-06	0.6188E-13	0.6458E-13	0.1000E-23	0.1252E-12	0.2191E-12	0.3132E-13	0.2381E-11	0.1349E-13	0.6307E-13
0.358	0.2827E+03	0.4155E-06	0.6180E-13	0.6510E-13	0.1000E-23	0.1253E-12	0.2193E-12	0.3080E-13	0.2387E-11	0.1343E-13	0.6343E-13
0.338	0.2828E+03	0.4237E-06	0.6161E-13	0.6551E-13	0.1000E-23	0.1250E-12	0.2187E-12	0.3009E-13	0.2394E-11	0.1334E-13	0.6375E-13
0.318	0.2829E+03	0.4319E-06	0.6132E-13	0.6566E-13	0.1000E-23	0.1240E-12	0.2169E-12	0.2916E-13	0.2400E-11	0.1317E-13	0.6397E-13
0.298	0.2830E+03	0.4399E-06	0.6094E-13	0.6538E-13	0.1000E-23	0.1220E-12	0.2135E-12	0.2800E-13	0.2407E-11	0.1291E-13	0.6404E-13
0.278	0.2830E+03	0.4476E-06	0.6052E-13	0.6445E-13	0.1000E-23	0.1180E-12	0.2079E-12	0.2659E-13	0.2415E-11	0.1252E-13	0.6391E-13
0.258	0.2831E+03	0.4548E-06	0.6009E-13	0.6266E-13	0.1000E-23	0.1141E-12	0.1997E-12	0.2495E-13	0.2422E-11	0.1198E-13	0.6350E-13
0.238	0.2832E+03	0.4613E-06	0.5971E-13	0.5985E-13	0.1000E-23	0.1077E-12	0.1885E-12	0.2311E-13	0.2428E-11	0.1127E-13	0.6278E-13
0.218	0.2832E+03	0.4670E-06	0.5939E-13	0.5599E-13	0.1000E-23	0.9963E-13	0.1744E-12	0.2112E-13	0.2434E-11	0.1040E-13	0.6174E-13
0.198	0.2833E+03	0.4719E-06	0.5916E-13	0.5129E-13	0.1000E-23	0.9037E-13	0.1582E-12	0.1910E-13	0.2439E-11	0.9411E-14	0.6047E-13
0.178	0.2834E+03	0.4759E-06	0.5903E-13	0.4627E-13	0.1000E-23	0.8081E-13	0.1415E-12	0.1721E-13	0.2443E-11	0.8399E-14	0.5910E-13
0.158	0.2835E+03	0.4789E-06	0.5899E-13	0.4170E-13	0.1000E-23	0.7232E-13	0.1267E-12	0.1563E-13	0.2447E-11	0.7505E-14	0.5788E-13
0.138	0.2837E+03	0.4810E-06	0.5900E-13	0.3848E-13	0.1000E-23	0.6642E-13	0.1163E-12	0.1459E-13	0.2450E-11	0.6885E-14	0.5704E-13
0.118	0.2839E+03	0.4822E-06	0.5900E-13	0.3735E-13	0.1000E-23	0.6437E-13	0.1127E-12	0.1423E-13	0.2454E-11	0.6669E-14	0.5600E-13

TCLOCK 1150.00 (0.319 HRS)
DT 5.00

GLEVL (KM) 0.118
WAGRID(1) -97.67

Z(KM)	HMSX-A1	HMSX-C	CLOUD	EXCAT-A1	HION-C	SO2-G	SO2-C	H2O2-G	H2O2-C	NO3-G	NO3-C
0.618	0.3333E-21	0.1000E-23	0.0000E+00	0.1344E-13	0.0000E+00	0.5935E-13	0.1000E-23	0.3142E-13	0.1000E-23	0.8902E-13	0.1000E-23
0.598	0.3981E-21	0.1000E-23	0.0000E+00	0.1347E-13	0.0000E+00	0.5948E-13	0.1000E-23	0.3148E-13	0.1000E-23	0.8922E-13	0.1000E-23
0.578	0.6299E-21	0.1000E-23	0.0000E+00	0.1350E-13	0.0000E+00	0.5966E-13	0.1000E-23	0.3156E-13	0.1000E-23	0.8949E-13	0.1000E-23
0.558	0.1161E-20	0.1000E-23	0.0000E+00	0.1353E-13	0.0000E+00	0.5988E-13	0.1000E-23	0.3164E-13	0.1000E-23	0.8983E-13	0.1000E-23
0.538	0.2270E-20	0.1000E-23	0.0000E+00	0.1356E-13	0.0000E+00	0.6013E-13	0.1000E-23	0.3174E-13	0.1000E-23	0.9022E-13	0.1000E-23
0.518	0.4485E-20	0.1000E-23	0.0000E+00	0.1359E-13	0.0000E+00	0.6041E-13	0.1000E-23	0.3183E-13	0.1000E-23	0.9066E-13	0.1000E-23
0.498	0.8749E-20	0.1000E-23	0.0000E+00	0.1362E-13	0.0000E+00	0.6070E-13	0.1000E-23	0.3191E-13	0.1000E-23	0.9114E-13	0.1000E-23
0.478	0.1666E-19	0.1000E-23	0.0000E+00	0.1364E-13	0.0000E+00	0.6099E-13	0.1000E-23	0.3197E-13	0.1000E-23	0.9165E-13	0.1000E-23
0.458	0.3081E-19	0.1000E-23	0.0000E+00	0.1367E-13	0.0000E+00	0.6128E-13	0.1000E-23	0.3200E-13	0.1000E-23	0.9217E-13	0.1000E-23
0.438	0.5515E-19	0.1000E-23	0.0000E+00	0.1370E-13	0.0000E+00	0.6153E-13	0.1000E-23	0.3197E-13	0.1000E-23	0.9269E-13	0.1000E-23
0.418	0.9543E-19	0.1000E-23	0.0000E+00	0.1373E-13	0.0000E+00	0.6172E-13	0.1000E-23	0.3187E-13	0.1000E-23	0.9319E-13	0.1000E-23
0.398	0.1594E-18	0.1000E-23	0.0000E+00	0.1376E-13	0.0000E+00	0.6185E-13	0.1000E-23	0.3166E-13	0.1000E-23	0.9361E-13	0.1000E-23
0.378	0.2570E-18	0.1000E-23	0.0000E+00	0.1380E-13	0.0000E+00	0.6188E-13	0.1000E-23	0.3132E-13	0.1000E-23	0.9391E-13	0.1000E-23
0.358	0.3991E-18	0.1000E-23	0.0000E+00	0.1384E-13	0.0000E+00	0.6180E-13	0.1000E-23	0.3080E-13	0.1000E-23	0.9399E-13	0.1000E-23
0.338	0.5966E-18	0.1000E-23	0.0000E+00	0.1387E-13	0.0000E+00	0.6161E-13	0.1000E-23	0.3009E-13	0.1000E-23	0.9373E-13	0.1000E-23
0.318	0.8574E-18	0.1000E-23	0.0000E+00	0.1322E-13	0.0000E+00	0.6132E-13	0.1000E-23	0.2916E-13	0.1000E-23	0.9297E-13	0.1000E-23
0.298	0.1183E-17	0.1000E-23	0.0000E+00	0.1317E-13	0.0000E+00	0.6094E-13	0.1000E-23	0.2800E-13	0.1000E-23	0.9151E-13	0.1000E-23
0.278	0.1563E-17	0.1000E-23	0.0000E+00	0.1302E-13	0.0000E+00	0.6052E-13	0.1000E-23	0.2659E-13	0.1000E-23	0.8911E-13	0.1000E-23
0.258	0.1975E-17	0.1000E-23	0.0000E+00	0.1265E-13	0.0000E+00	0.6009E-13	0.1000E-23	0.2495E-13	0.1000E-23	0.8557E-13	0.1000E-23
0.238	0.2382E-17	0.1000E-23	0.0000E+00	0.1203E-13	0.0000E+00	0.5971E-13	0.1000E-23	0.2311E-13	0.1000E-23	0.8076E-13	0.1000E-23
0.218	0.2739E-17	0.1000E-23	0.0000E+00	0.1109E-13	0.0000E+00	0.5939E-13	0.1000E-23	0.2112E-13	0.1000E-23	0.7472E-13	0.1000E-23
0.198	0.3000E-17	0.1000E-23	0.0000E+00	0.9871E-14	0.0000E+00	0.5916E-13	0.1000E-23	0.1910E-13	0.1000E-23	0.6777E-13	0.1000E-23
0.178	0.3172E-17	0.1000E-23	0.0000E+00	0.8379E-14	0.0000E+00	0.5903E-13	0.1000E-23	0.1721E-13	0.1000E-23	0.6061E-13	0.1000E-23
0.158	0.3242E-17	0.1000E-23	0.0000E+00	0.6558E-14	0.0000E+00	0.5899E-13	0.1000E-23	0.1563E-13	0.1000E-23	0.5424E-13	0.1000E-23
0.138	0.3258E-17	0.1000E-23	0.0000E+00	0.4459E-14	0.0000E+00	0.5900E-13	0.1000E-23	0.1459E-13	0.1000E-23	0.4982E-13	0.1000E-23
0.118	0.3260E-17	0.1000E-23	0.0000E+00	0.2141E-14	0.0000E+00	0.5908E-13	0.1000E-23	0.1423E-13	0.1000E-23	0.4827E-13	0.1000E-23

TCLOCK 1150.00 (0.319 HRS)
DT 5.00

GLEVL (KM) 0.118
WAGRID(1) -97.67

Z (KM)	NO3-A1	NH4-G	NH4-C	NH4-A1	KFORM-G	KFORM-C	KEXAN-1	KEXAN-2	P	CS
0.618	0.2967E-13	0.5935E-13	0.1000E-23	0.1484E-12	0.5935E-13	0.1000E-23	0.1344E-13	0.1344E-13	0.7796E+06	0.3335E-04
0.598	0.2974E-13	0.5948E-13	0.1000E-23	0.1487E-12	0.5948E-13	0.1000E-23	0.1347E-13	0.1347E-13	0.7815E+06	0.3341E-04
0.578	0.2983E-13	0.5966E-13	0.1000E-23	0.1492E-12	0.5966E-13	0.1000E-23	0.1350E-13	0.1350E-13	0.7834E+06	0.3347E-04
0.558	0.2994E-13	0.5988E-13	0.1000E-23	0.1497E-12	0.5988E-13	0.1000E-23	0.1353E-13	0.1353E-13	0.7853E+06	0.3353E-04
0.538	0.3007E-13	0.6015E-13	0.1000E-23	0.1504E-12	0.6015E-13	0.1000E-23	0.1356E-13	0.1356E-13	0.7872E+06	0.3360E-04
0.518	0.3022E-13	0.6044E-13	0.1000E-23	0.1511E-12	0.6045E-13	0.1000E-23	0.1359E-13	0.1359E-13	0.7891E+06	0.3366E-04
0.498	0.3038E-13	0.6076E-13	0.1000E-23	0.1519E-12	0.6077E-13	0.1000E-23	0.1362E-13	0.1362E-13	0.7910E+06	0.3373E-04
0.478	0.3055E-13	0.6110E-13	0.1000E-23	0.1527E-12	0.6112E-13	0.1000E-23	0.1364E-13	0.1364E-13	0.7929E+06	0.3380E-04
0.458	0.3072E-13	0.6145E-13	0.1000E-23	0.1536E-12	0.6149E-13	0.1000E-23	0.1367E-13	0.1367E-13	0.7949E+06	0.3387E-04
0.438	0.3090E-13	0.6180E-13	0.1000E-23	0.1545E-12	0.6188E-13	0.1000E-23	0.1370E-13	0.1370E-13	0.7968E+06	0.3394E-04
0.418	0.3106E-13	0.6213E-13	0.1000E-23	0.1553E-12	0.6227E-13	0.1000E-23	0.1373E-13	0.1373E-13	0.7987E+06	0.3401E-04
0.398	0.3120E-13	0.6241E-13	0.1000E-23	0.1560E-12	0.6267E-13	0.1000E-23	0.1376E-13	0.1376E-13	0.8007E+06	0.3408E-04
0.378	0.3130E-13	0.6261E-13	0.1000E-23	0.1565E-12	0.6307E-13	0.1000E-23	0.1380E-13	0.1380E-13	0.8026E+06	0.3415E-04
0.358	0.3133E-13	0.6266E-13	0.1000E-23	0.1567E-12	0.6343E-13	0.1000E-23	0.1384E-13	0.1384E-13	0.8045E+06	0.3422E-04
0.338	0.3124E-13	0.6249E-13	0.1000E-23	0.1562E-12	0.6375E-13	0.1000E-23	0.1387E-13	0.1387E-13	0.8065E+06	0.3430E-04
0.318	0.3099E-13	0.6198E-13	0.1000E-23	0.1550E-12	0.6397E-13	0.1000E-23	0.1322E-13	0.1322E-13	0.8084E+06	0.3437E-04
0.298	0.3050E-13	0.6101E-13	0.1000E-23	0.1525E-12	0.6404E-13	0.1000E-23	0.1317E-13	0.1317E-13	0.8104E+06	0.3444E-04
0.278	0.2970E-13	0.5941E-13	0.1000E-23	0.1485E-12	0.6391E-13	0.1000E-23	0.1302E-13	0.1302E-13	0.8123E+06	0.3452E-04
0.258	0.2852E-13	0.5706E-13	0.1000E-23	0.1426E-12	0.6350E-13	0.1000E-23	0.1265E-13	0.1265E-13	0.8143E+06	0.3459E-04
0.238	0.2692E-13	0.5385E-13	0.1000E-23	0.1346E-12	0.6278E-13	0.1000E-23	0.1203E-13	0.1203E-13	0.8163E+06	0.3467E-04
0.218	0.2491E-13	0.4983E-13	0.1000E-23	0.1246E-12	0.6174E-13	0.1000E-23	0.1109E-13	0.1109E-13	0.8182E+06	0.3475E-04
0.198	0.2259E-13	0.4520E-13	0.1000E-23	0.1130E-12	0.6047E-13	0.1000E-23	0.9871E-14	0.9871E-14	0.8202E+06	0.3482E-04
0.178	0.2020E-13	0.4043E-13	0.1000E-23	0.1011E-12	0.5910E-13	0.1000E-23	0.8379E-14	0.8379E-14	0.8222E+06	0.3489E-04
0.158	0.1808E-13	0.3619E-13	0.1000E-23	0.9047E-13	0.5788E-13	0.1000E-23	0.6558E-14	0.6558E-14	0.8242E+06	0.3496E-04
0.138	0.1661E-13	0.3324E-13	0.1000E-23	0.8310E-13	0.5704E-13	0.1000E-23	0.4459E-14	0.4459E-14	0.8262E+06	0.3503E-04
0.118	0.1609E-13	0.3221E-13	0.1000E-23	0.8053E-13	0.5680E-13	0.1000E-23	0.2141E-14	0.2141E-14	0.8282E+06	0.3509E-04

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