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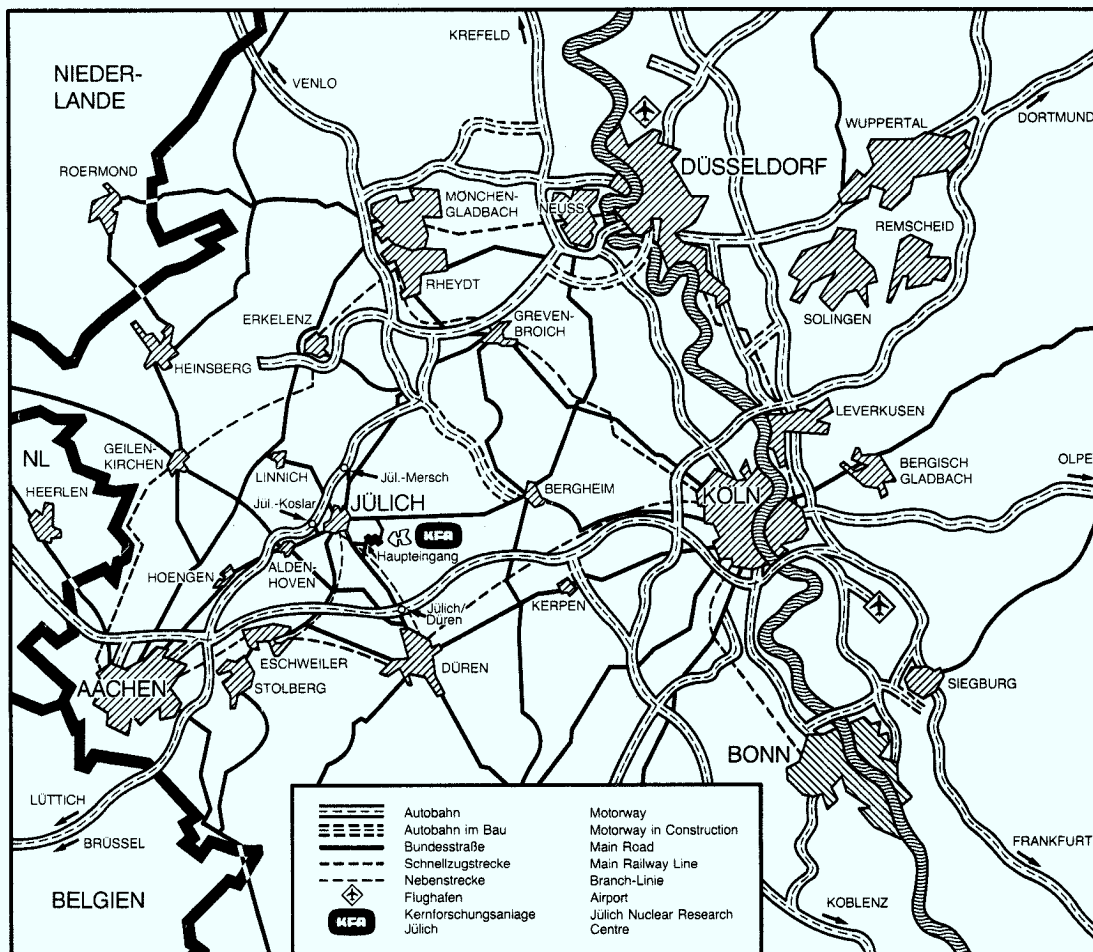
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**Description of a One-Dimensional Model
for Atmospheric Chemistry**

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Description of a One-Dimensional Model for Atmospheric Chemistry

by

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1. Introduction

The purpose of atmospheric modelling is to describe the physical and chemical state of the earth's atmosphere as exactly as possible. In order to do so, one has to consider the basic laws of energy and momentum conservation, the mass continuity equation and the equations of radiative transfer. With these equations it is - in principle - possible to describe atmospheric conditions exactly. In practice, however, one has to make a number of simplifications since the available computer facilities, especially the limited storage, running time and costs, are inadequate. (E.g.: Miller et al., 1979; Tuck, 1979; Lin et al., 1980; Pyle, 1980; Pyle and Rogers, 1980; Garcia and Solomon, 1983).

The purpose of the one-dimensional model presented here is to describe the chemical behaviour and the concentration profiles of atmospheric gases. Therefore we only have to consider the mass continuity equation and neither the equation for momentum continuity nor that for conservation of energy are taken into account. They are instead implicitly defined by boundary conditions. Concerning the radiative transfer, we have to make a number of assumptions described below.

Solving the mass continuity equations for all the components of the atmosphere leads to a time-dependent model, three-dimensional in space. If we reduce the geometrical dependencies by averaging over longitude and, furthermore, over latitude, we obtain a time-dependent, one-dimensional (1-D) model, by means of which globally averaged profiles of concentrations with altitude are attained.

Our 1-D-model lays great emphasis on the chemical behaviour of the atmosphere. The program allows three different versions.

It is valid for describing the natural background atmosphere, to estimate long-term, anthropogenic perturbations of the chemical steady-state and a short-term version helps to understand the diurnal variations of the components.

As we try to describe the chemical behaviour of the atmosphere, we have to include all relevant components identified up to now as well as those which must necessarily be there, inspite of the fact that their concentrations are too small to be measured. Altogether we are considering about fifty different species listed in Table 1.

Table 1a: List of long-lived species and standard boundary values used in the one-dimensional model system. At the lower boundary, either mixing ratios $X(0)$ or deposition velocities $V(0)$ and production fluxes $Prod(0)$ are used. At the upper boundary, mixing ratios $X(100)$ are inserted throughout.

X(0)	V(0)	Prod.(0)	X(100)	Substance
2.00E-10	1.50E-01	0.00	3.40E-03	O _{odd}
1.50E-11			1.00E-10	N _{odd}
			1.00E-07	H _{odd}
	8.00E-01	1.10E+10	9.00E-12	SO _x
	1.00E-01	1.50E+08	1.00E-60	H _x S
	0.00	0.00	2.50E-09	ClO _x
	0.00	0.00	1.00E-20	CH _x O _y
3.30E-07			2.50E-11	N ₂ O
	0.00	8.00E+03	1.00E-40	NH ₃
	0.00	0.00	1.00E-40	NH ₄ ⁺
	5.00E-01	0.00	1.00E-16	HNO ₃
5.50E-07			5.00E-07	H ₂
8.60E-03			4.00E-06	H ₂ O(g)
	0.00	0.00	0.00E+00	H ₂ O(l)
5.00E-10			1.00E-10	H ₂ O ₂
5.00E-10			9.00E-12	H ₂ SO ₄
5.00E-10			1.00E-40	COS
1.10E-07			3.30E-07	CO
3.32E-04			2.70E-04	CO ₂
1.66E-06			2.00E-08	CH ₄
2.50E-10			1.00E-18	C ₂ H ₂
2.00E-09			1.00E-35	C ₂ H ₆
3.00E-10			1.00E-45	C ₃ H ₈
1.90E-10			1.00E-25	CCl ₃ F
3.20E-10			1.00E-15	CCl ₂ F ₂
1.25E-10			1.00E-35	CCl ₄
6.50E-10			6.70E-24	CH ₃ Cl
4.50E-11			1.00E-40	CHCl ₃
1.65E-10			1.00E-18	CH ₃ CCl ₃
1.50E-10			1.70E-10	HCl

NO_x-Production by lightning: 5.92E+08cm⁻²s⁻¹ around 4.5 km

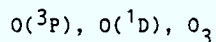
by aircrafts: 8.00E+07cm⁻²s⁻¹ around 10.0 km

SO₂-Production by vulcanoes: 2.15E+08cm⁻²s⁻¹ around 1.5 km

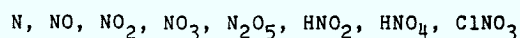
This model description addresses mainly the expert, whom we want to explain how we are solving the special problems of our field. Therefore the algorithms are explained in full detail and an extended appendix is added. The first chapters, however, introduce the general aspects of atmospheric modelling and the philosophy behind our model especially.

Table 1b: List of short-lived species which are calculated (besides within the shortterm version) assuming steady-state conditions

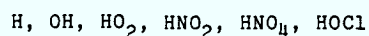
Oxygen particles:



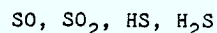
Nitrogen containing species:



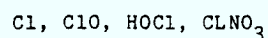
Compounds of hydrogen:



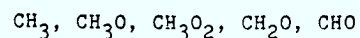
Sulphur containing substances:



Chlorine species:



Organic radicals:



2. General Description of the Model

2.1 Basic Equations

Besides field experiments on the composition of the earth's atmosphere and laboratory investigations about the chemical reactions of the species, abundant in the air, model calculations are necessary to describe the chemistry of the atmosphere. The atmospheric models are mathematical formulations of the theory of the atmosphere and contain solutions of the basic differential equations, which characterize the physical and chemical state of the atmosphere.

The behavior of the atmosphere is described by the continuity equations for energy, momentum and mass. As all actions within the atmosphere are driven by the solar energy, the laws of the radiative transport have to be included to characterize the distribution of the energy.

There are only a limited number of basic equations, but the obstacles become apparent, if one tries to explain the actions of the atmosphere quantitatively. E.g., it isn't sufficient to know that the energy content of the system "atmosphere" is constant, but one has to be aware how much of the sun's energy is present at the different locations within the atmosphere. And it must be known in dependence of the energy distribution.

The momentum continuity equation is transformed in the models into a detailed record of the movement of the air parcels and its dependence on time and location.

Concerning a chemical model of the atmosphere, the most important law is the mass continuity equation. The net change of the concentration C_i of each constituent i , according to time t at a certain point in space is given by the equation

$$\frac{\partial C_i}{\partial t} = P_{jk} - D_i \cdot C_i + TT_i$$

which contains a production term $P_{jk}(z)$, depending on the reacting components j, k other than i , a destruction term $D_i(z) \cdot C_i(z)$ proportional to the concentration of the component i and a transport term TT_i , which in a 1-D-model describes the transport through a layer of thickness dz at an altitude z . For a globally averaged model, this transport can be treated as a vertical eddy-diffusion given by

$$TT_i = \frac{\partial}{\partial z} \left[K_z \cdot M \frac{\partial (C_i/M)}{\partial z} \right]$$

where $M(z)$ is the total concentration of air at a given altitude and $K(z)$ is the so-called eddy-diffusion coefficient (see below), a model parameter depending only on the altitude z and tuned to fit the altitudinal profile of the trace gas.

The production rate $P_{jk}(z)$ and the destruction frequency $D_i(z)$ of a species are both time-dependent because they contain other constituents j, k, l of the atmosphere which depend on time and location. In general, these terms can be split into three parts, one describing the gas-phase reactions and the second the photo-dissociations. The last one deals with heterogeneous reactions, which in the case of our model are restricted to wet chemistry:

$$P = P_{\text{gas}} + P_{\text{photo}} + P_{\text{wet}}$$

$$D = D_{\text{gas}} + D_{\text{photo}} + D_{\text{wet}}$$

The atmosphere is not a closed system and, therefore, the manifold interactions with the biosphere, hydrosphere and lithosphere enter into the description of its behavior. And the continuity equations for the energy, the momentum and

the mass are present in the form of differential equations which means, that boundary conditions are an essential part of the mathematical algorithms.

For a one-dimensional, photochemical model this means, that boundary conditions both, in space and in time, have to be defined or a steady-state assumption, where the time dependence vanishes, must be regarded.

2.2 Problems of Model Calculations

The mathematical tools necessary to solve the differential system of mass continuity equations are available and common to all modellers. The accuracy of the algorithms are predictable and the numerical errors of every computer are well known. Therefore the only mathematical problems are linked to the search for appropriate algorithms.

As said above, all models need boundary conditions and other input parameters, e.g. the rate constants for chemical reactions. All these data possess either a natural variation like the deposition velocities or the sun's radiance, or they are only known within a certain error range. But these errors and variations can be taken into account in the model results.

Much worse than these well known facts are errors which are not predictable, like missing reactions and other systematical errors. Therefore the models have to be validated by comparing their results to the findings of field measurements.

But here the problems spring up. Every model calculation is dealing with averaged values, but field experiments only give data specific for time and location. To compare both, one has to apply the same averaging procedures to the field data as are used in the model algorithms. Unfortunately the number of field data is far too limited to allow such validation.

For long lived species there are more or less sufficient data, especially those gained from satellite observations. But these components of the air are not very useful for the validation, as they are not reactive and therefore more dependent on physical processes than on chemical ones.

On the other hand, the non-inert particles, the radicals, are very difficult to observe and we need a lot of measurements as they are very much dependent on location and time. Nowadays the temporary reservoir gases, e.g. ClNO_3 , H_2O_2 , N_2O_5 , HNO_4 , HOCl , which are formed by recombination of two radicals, play a key role in the validation. They are quite instable, but their concentrations are big enough, so that it should be possible to measure them.

The main criteria for the validation of model calculations are the comparisons of local and time-dependent trends. By these comparisons one is able to find out whether all appropriate chemical reactions are included in the models. This can be done particularly if related constituents of the atmosphere are observed simultaneously.

2.3 The Parameters

As our model is restricted to consider only the mass continuity equation, the other fundamental laws have to be taken into account via parameters, which are kept constant during one run of the program. These parameters, which have to be read in, are the concentration of air, the temperature profile and the eddy-diffusion coefficient profile, respectively. For concentration of air and the temperature profile, we use the data given by Cole and Kantor (1979). To obtain a reasonable, model consistent annual average, we applied the same averaging procedure to these values, as we used to derive the eddy diffusion coefficient (Janßen-Schmidt, 1981). Air concentration, temperature and eddy coefficient are plotted in figure 1.

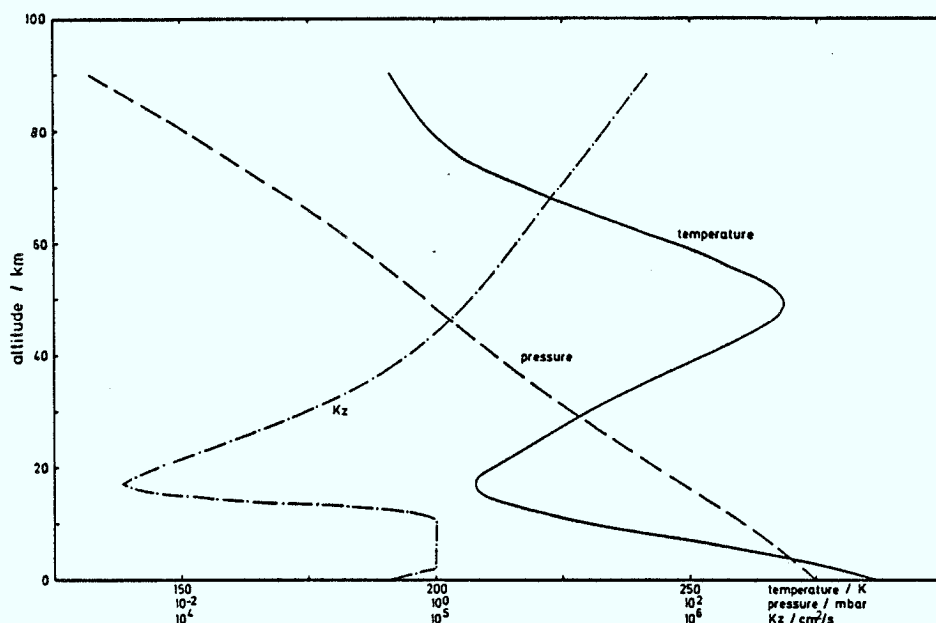


Figure 1: Altitudinal dependency of temperature (—), pressure (---) and eddy-diffusion coefficient K_z (-.-)

Besides these profiles, we need the reaction constants for the gas-phase and the wet chemistry, as well as the solar flux, the absorption cross-sections and the quantum yields for calculating the photochemical reaction rates. The data used are listed in the tables of appendix A.2 and A.3. In most cases these data are the recommended values. The solar flux is from Ackermann (1971) modified by means of the data given by Simon (1976).

As the equation to be solved is a second-order differential equation in space, two boundary conditions have to be added to the set of equations which describe the altitudinal profiles of the constituents. We apply fixed mixing ratios at the upper boundary and either fixed fluxes (production rates and deposition velocities) or fixed mixing ratios at the lower

boundary. The normal range for the altitude is from 0 km to 99 km, but as we do not include ion chemistry, the profiles are valid only up to 65 km. The range between 65 and 99 km is applied to make sure that the errors of the 99 km boundary values will not propagate down to our actual range. This can be ascertained by using rather low values for these data, as the error then cannot exceed 100 %, whereas too high values may introduce much bigger errors. This fact was varified by a series of testing runs.

Besides the boundary conditions, there are no more restrictions to the concentration profiles. In fact, we use physically plausible conditions like constant mixing ratios for CO_2 or for the total amount of H or Cl atoms to prove that the mathematical treatment is correct and that there are no numerical errors in the procedure.

Additional boundary conditions for the time-dependent versions of the model are the starting profiles for all the components. We get these profiles from a preceding run of the steady-state version.

Besides these parameters, necessary for the calculation itself, there are others which influence the course of the program. Such parameters are e.g. switches which allow calculations with and without clouds, or those governing the different various of the model or additional output routines. These program parameters are described in the program listings.

2.4 Specialities of the KFA-Model

The model developed at the Kernforschungsanlage Jülich (KFA), which is described here, is designed to support the field experiments done by the Institute for Atmospheric Chemistry of the KFA. Therefore great emphasis was laid to build a program readable for non-modellers, too. In subprogram CHEMIE

for example a standard assignment for the production rates and destruction frequencies of all species is used. So, if there is no production for a constituent, the production rate is expressively set equal zero, to demonstrate this fact. We preferred to enlarge the necessary storage rather than to eliminate those data, which are not used in the course of the program.

A second scheme followed in this model is that all data, either input or output or intermediate, are easily to be extracted by means of built-in print or plot routines. To avoid unnecessary large outputs, we separated the output program from the calculation. The main program itself only prints out the starting parameters and the final output of the concentrations. All other data are written onto a peripheral mass storage from which the print-out program reads the data and creates a separate listing of the data wanted. The print-out program, too, prepares the data for the plots.

Besides this way of adding output to the standard values, several subroutines can be activated by steering parameters. So it is possible, e.g. to list and to plot the rates of every single reaction, either absolutely or relatively to the overall production or destruction rate for a specific constituent. Another subroutine prints out the mixing ratio for a constituent, chosen via input parameters, at every minute for a full daily cycle.

As for the spectral data the photon fluxes and the photodissociation frequencies used in the model can be printed out via the peripheral mass storage. An additional program, which uses the same input routine and the same subroutine as the main model, is applied if special outputs of spectral parameters are derived. With this program it is possible to calculate the photon fluxes and the photodissociation frequencies in dependence of the solar zenith angle or to

get a separate print-out for the photon flux from above and below a horizontal plane.

An additional advantage of the clearly and distinctly written program and the large amount of output possibilities is the fact, that special runs are easily done. So it is possible, e.g. to eliminate reaction for one species, but not for others, to find out the effect of the reaction for this component. Or one or more constituents can be kept constant, if measured data for these species are available, to simulate special experimental conditions. Altogether, the main purpose of the KFA model is to support the field experiments rather than to do model development.

As the tropospheric chemistry is not included in full detail in the model and as the planetary boundary layer is not considered at all, the model is mainly valid for the stratosphere. The data given for the tropospheric altitude range are valid only for the free troposphere within the limitations of the reaction system applied.

3. Radiative Flux and Photochemistry

3.1 The Photon Flux through the Atmosphere

As the flux of photons from the sun provides the atmosphere with the energy necessary to maintain chemical processes, great emphasis is laid on calculating the solar flux. Indeed, this is the most time-consuming part of our model.

The flux of photons emitted by the sun depends on the wavelength according to the black body radiation theory. We use the values for the solar radiance given by Ackermann (1971) and modified by Simon (1976), as shown in figure 2.

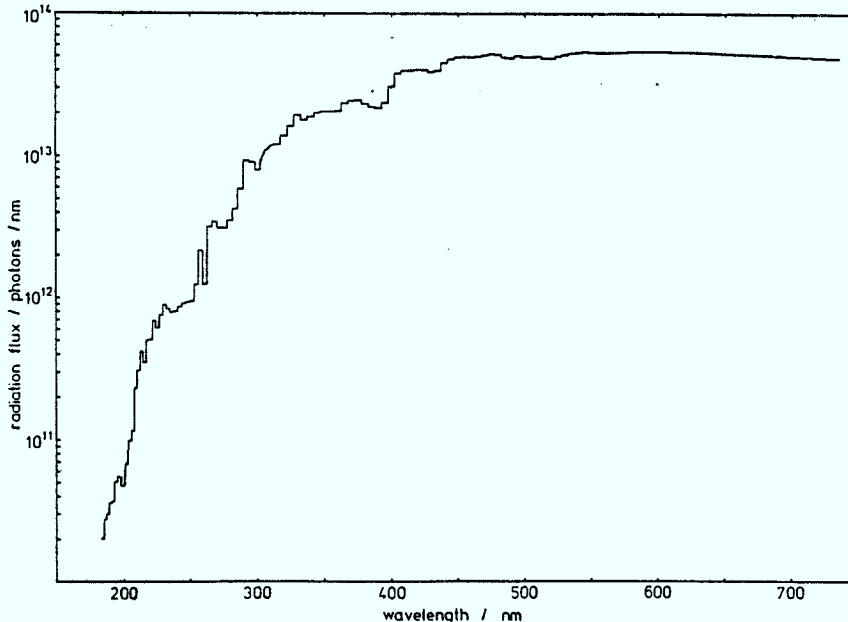


Figure 2: Wavelength dependency of the solar photon flux according to Ackerman (1971) and Simon (1974). The steps represent the wavelength intervals for which the calculation is done.

While proceeding through the atmosphere, the photons interact with the different components of the air. At altitudes covered by our calculations, the dominant processes changing the amount of photons are absorption by molecular oxygen (O_2), ozone (O_3) and nitrogendioxide (NO_2), Rayleigh-scattering at air molecules and surface and cloud albedos. Mie-scattering at aerosols is important, too, but due to the lack of information about aerosol layers, we declined to include this scattering.

When light passes through an absorbing medium, the flux is diminished according to the Lambert-Beer's law:

$$\frac{dF^\lambda}{ds} = -\sigma^\lambda \cdot C \cdot F^\lambda$$

or integrated:

$$F^\lambda = F_0^\lambda e^{-\sigma^\lambda C s}$$

where F is the wavelength-dependent flux intensity and σ the absorption cross-section of the absorber, whose concentration is given by C . The path-length of the light within the medium is defined by s and λ represents the wavelength.

As the concentration of the absorbing species in the atmosphere is not homogeneous, the total flux at an altitude z_0 in a purely absorbing medium is given by

$$F^\lambda = F_0^\lambda \exp \left[\sum_{i=1}^n \int_{z_0}^{\infty} \sigma_i^\lambda C_i(s) ds \right]$$

i numerates the different absorbing constituents in the atmosphere. Assuming a plane parallel atmosphere, the integral can be evaluated by:

$$\int_{z_0}^{\infty} \sigma_i^\lambda C_i(s) ds = \sigma_i^\lambda \int_{z_0}^{\infty} C_i(z) \sec \theta(t) dz = \sigma_i^\lambda \tau_i$$

where θ is the zenith angle, depending on the time t and on the geographical location and z is the altitude. τ_i is the so-called optical depth of the absorber i .

If the curvature of the earth is taken into account, the above formula has to be modified by a factor, known as Chapman function (see e.g. Craig, 1965). Besides being absorbed, the radiance might be scattered at air molecules, i.e. it might undergo Rayleighscattering. This scattering can be expressed by the Rayleighscattering cross-section:

$$\sigma_R = \frac{8\pi^3(n_s^2 - 1)^2}{3\lambda^4 C_{air}^s} \left[\frac{6+3\varrho_n}{6-7\varrho_n} \right]$$

where n_s is the refraction-index of air at 1013 mbar pressure and 15 °C temperature. C_{air}^s is the concentration of air at the same conditions and ϱ_n is the depolarization factor ($0 \leq \varrho_n \leq 0.5$). The factor $[6+3\varrho_n/6-7\varrho_n]$ describes the influence of the optical anisotrope molecules. For air, ϱ_n is equal to 0.035 (Gucker u. Basu, 1953).

As the photon may undergo molecular scattering several times, the exact calculation of the Rayleigh-scattering is a very time-consuming matter and therefore it has to be simplified (Luther et al., 1978). The method we use to calculate multiple molecular scattering is based on the concept developed by Isaksen et al (1976). It is assumed that, on an average, the photons are either scattered in the direction of the solar flux or against it. The ratio for both directions is 1/2 to 1/2. By examining Isaksen's formula, we found that the expression for the scattered flux forms a converging series with a finite summation value as shown in appendix A1.3. With these assumptions, one gets fairly good agreement with the exact calculations carried out by Luther a. Gelinas (1975) as shown in fig. 3.

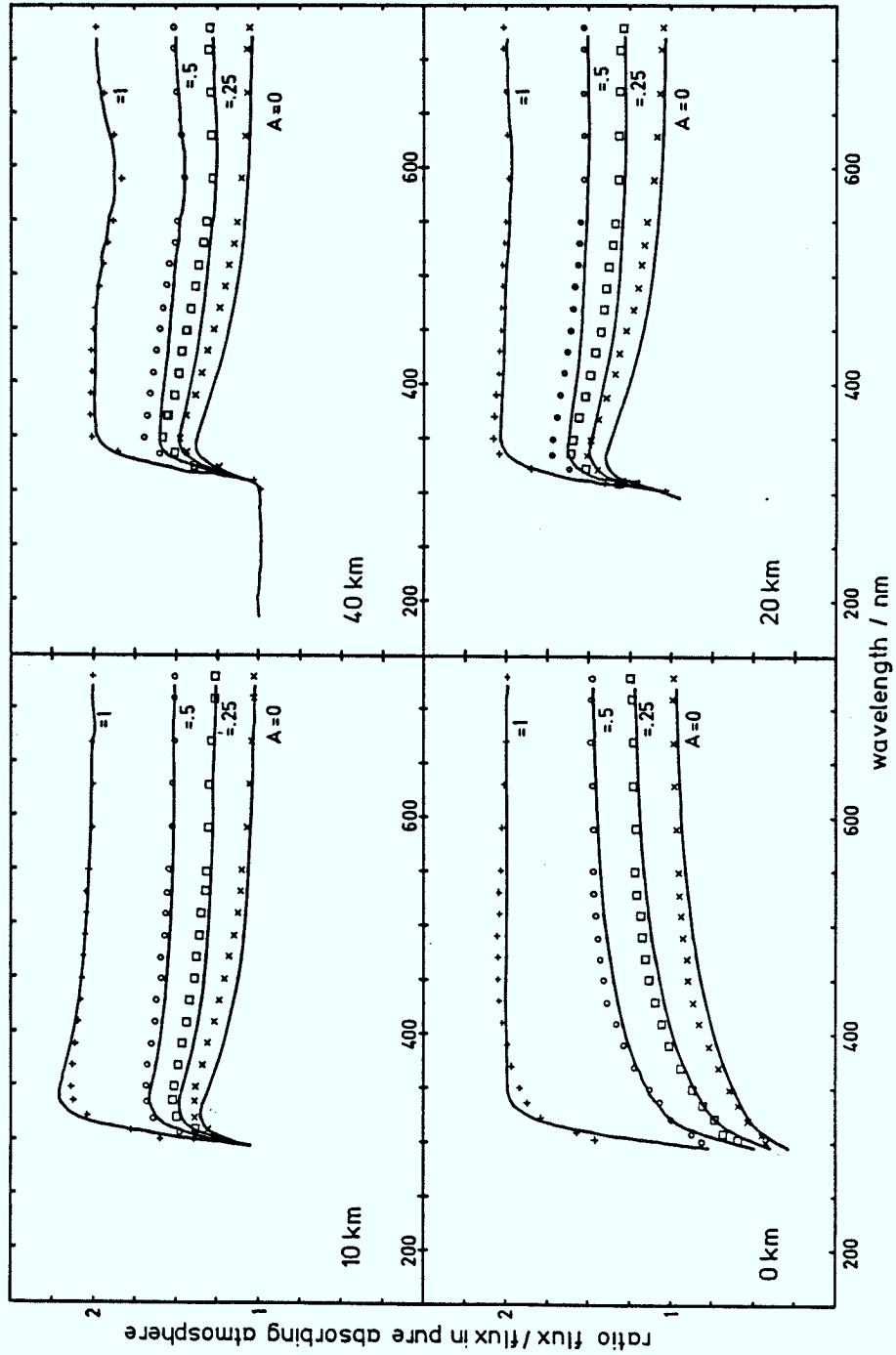


Figure 3: The influence of ground albedo A and the Rayleigh-scattering at different altitudes. The ratio of the flux including molecular scattering to the flux within a pure absorbing atmosphere is plotted versus wavelength. The points (*) represent the data of Luther and Gelinas (1975).

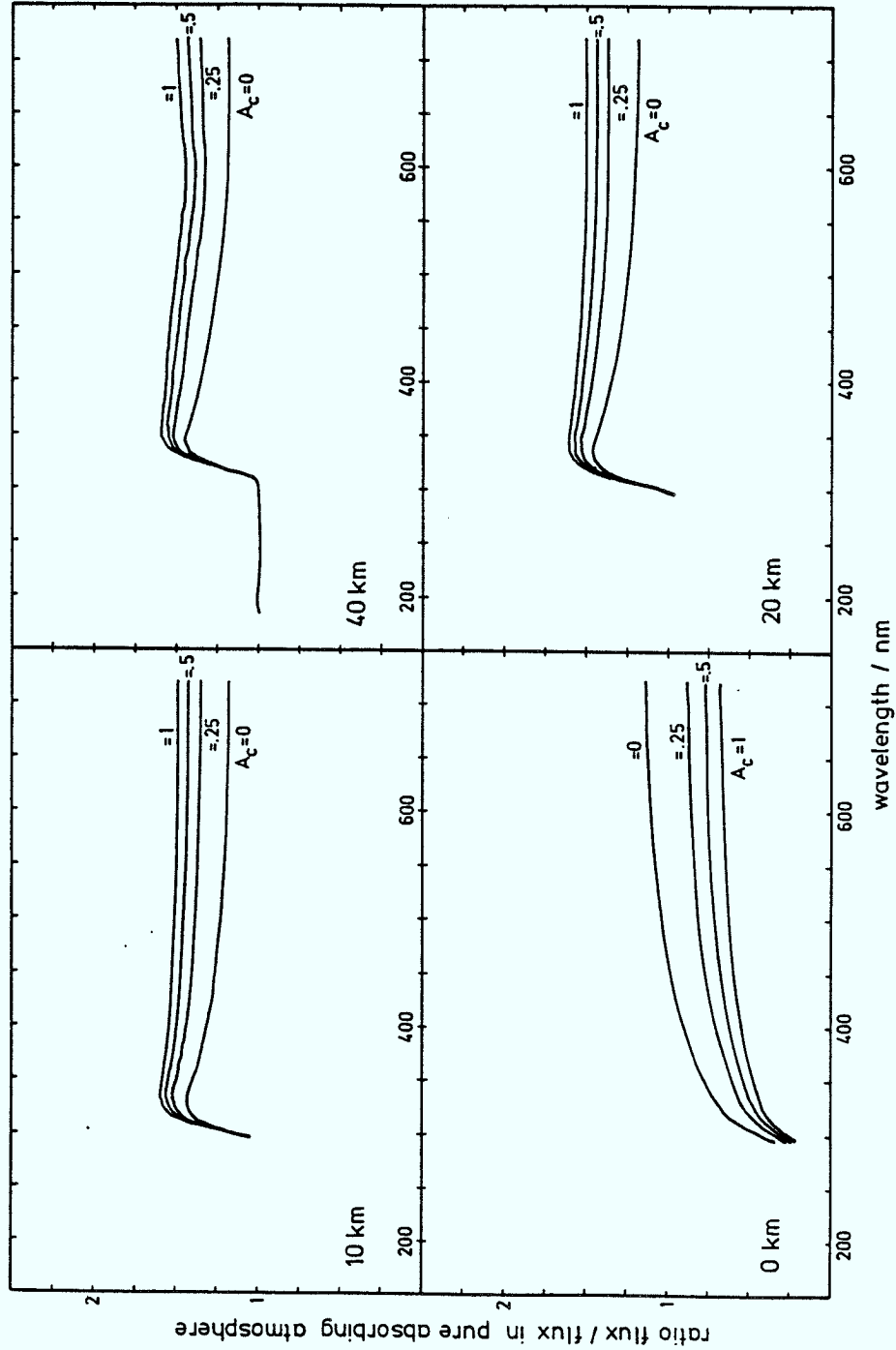


Figure 4: The influence of cloud albedo A_c and Rayleigh-scattering at different altitudes. The ratio plotted is the same as in figure 3. For all cases the ground albedo was set equal 0.167.

In figure 3, the reflectivity of the surface, i.e. the albedo, is changed, too. Actually the albedo is experimentally defined as the ratio of the amount of photons reaching the surface to the amount scattered backwards. In model calculations this is simulated by the reflectivity of the ground. The portion of the reflected light depends strongly on the nature of surface. In the model described here, we neglect the wavelength dependence of the albedo. As a globally averaged value we use 0.17 (Baumgartner et al., 1976). The cloud albedo is taken into account by introducing a cloud cover $HKT(z)$ depending on the altitude z (see appendix A1.3 and fig. 5). Normally we use an averaged cloud cover of 0.5 as obtained from measurements.

$$HKT(z) = 0.121 \exp(0.256z - 0.0436z^2)$$

For special calculations, e.g. in the short-term version of the model, we assume a single cloud at an altitude z_0 , given by

$$HKT(z) = A \frac{a}{\pi} e^{-a^2(z-z_0)^2}$$

with a cloud cover factor A . For the cloud albedo, we attain a value of 0.75. The influence of the cloud albedo for different cases is demonstrated in figure 4.

3.2 The Calculations of Photodissociation Coefficients

Every particle whether gaseous, liquid or solid has a characteristic absorption spectrum from which the cross-section for the interaction between the particle and a photon of defined energy can be obtained. For the atmospheric chemistry, the absorption cross-sections in the UV and visible region of the spectrum are most important as those photons will cause

a breaking up of molecular bonds, i.e. the photodissociation process. The cross-sections used for our model are depicted in appendix A.3.

If the photon flux $F(z)$ at a given altitude z is known, the photodissociation rate can be calculated from the absorption cross-section σ_i and the quantum yield ϕ_j^λ for the process j considered:

$$V_{ij}^{\text{photo}}(z) = \gamma_{ij}(z) C_i(z)$$

with a rate coefficient

$$\gamma_{ij}(z) = \int_{\lambda} \sigma_i^\lambda \cdot \phi_j^\lambda \cdot F^\lambda(z) d\lambda$$

Normally there is a threshold for the dissociation process, depending on the dissociation energy of the molecule. This threshold is not a sharp boundary; we, therefore, use a Fermi-function to describe the quantum yield:

$$\phi_i^\lambda = \frac{1}{\exp\left(\frac{\lambda - \lambda_0}{\Delta\lambda}\right) + 1}$$

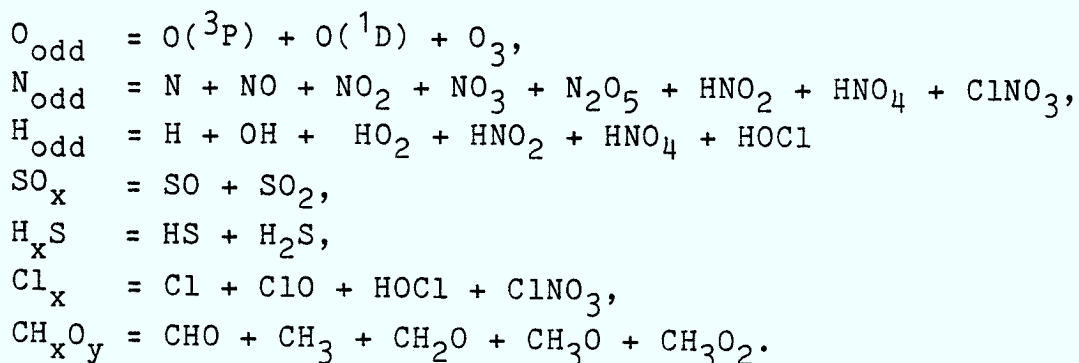
where λ_0 indicates the threshold and $\Delta\lambda$ defines the slope of the Fermi-function. The parameters of the quantum yields are also listed in appendix A.3. The use of a fermi-function is valid within the error bars of the experimental data, even for the best measurements.

4. Atmospheric Chemistry

4.1 Treatment of Gasphase Chemistry

A lot is known about the interactions between particles found or presumed to be present in the earth's atmosphere (DeMore et al., 1985, Baulch et al., 1982). But it is not necessary to calculate all the rates of the reactions occurring. This would be a very time-consuming job and therefore we have divided the reactions into three groups: the important ones, contributing by more than 3 % at any altitude to the overall production or destruction rate of a constituent, the less important, contributing by between 0.1 % and 3 % and the unimportant reactions, which contribute by less than 0.1 % to the overall rates. The unimportant reactions are not considered at all, whereas the less important are marked by the reaction number. That makes it easy to reduce the chemistry by just removing a few statements from subprogram CHEMIE, where the overall rates are calculated.

Considering the species, there is a critical parameter, which divides them into two groups. This parameter is the time required for the diffusion from one layer of thickness z to the neighboring ones. If the overall rate for production or destruction is small compared to this time, these components have to be calculated separately, whereas the reactive radicals can be grouped together. Within these groups, the exchange rate is rather large, but the group itself has small overall rates. These groups, within which steady-state is assumed, are:



As mentioned above, the overall production rates and destruction frequencies, i.e. the destruction rates divided by the concentration of the specific component, are calculated simultaneously for each altitude within the subprogram CHEMIE. To achieve true steady-state conditions within the groups, the exchange rates are calculated by three iterations. For the members of a group the concentration-ratios are calculated within the subprogram CHEMIE, keeping the concentration of the whole group constant. After solving the differential equation in space with the subprogram GAUSS for the steady-state version, or the differential equation in time by means of the subprogram EULER for the time-dependent versions, the concentrations of the group members are calculated according to the new overall concentration, now keeping the ratios within the group constant. To reduce the amplitude of oscillations from one iteration to the other (in the case of the steady-state version), a damping term was introduced by averaging the new and the old concentrations for all long-lived species.

4.2 Treatment of Wet Removal

While the gasphase interactions are directed reactions with educts and products, the dissolving process of gaseous particles in rain or cloud droplets normally occurs via an equilibrium, the direction depending on the amount of water present. That means, that the wash-out or rain-out of gasphase components from the atmosphere is closely connected to the concentration of liquid water in the air and to its' change with time.

In the stratosphere, the water vapour content depends on chemical reactions, mainly due to the reactions of OH with HO_2 , H_2 , CH_4 and CH_2O for the sources of H_2O , and the sinks are the photodissociation and the reaction with $\text{O}(^1\text{D})$ atoms. But in the troposphere chemical reactions are of minor influence as compared to evaporation and condensation. To

calculate the water vapour concentration, we use a fixed, globally averaged humidity profile shown in figure 5. Via the Clausius-Clapeyron equations for both water and ice

$$\ln p_{H_2O} = -\frac{\Delta H_{ice} + \Delta H_{water}}{RT} + \frac{\Delta S_{ice} + \Delta S_{water}}{R}$$

the concentration of gaseous water is a function of temperature and relative humidity. The enthalpy H and the entropy S of water has to be multiplied by a factor f whereas those of ice by a factor $(1-f)$. The factor f stands for the ratio of liquid water to the sum of water and ice:

$$f = \frac{[water]}{[water] + [ice]} = \frac{1}{\exp[2(z-8)] + 1}$$

If we now assume that the chemistry can be neglected in the troposphere, we obtain

$$\frac{\partial [H_2O]}{\partial t} = (-k_c [H_2O] + k_e [water]) + \frac{\partial}{\partial z} [K_z M \frac{\partial [H_2O]}{\partial z}]$$

for the continuity equation of water vapour (H_2O). k_c is the rate coefficient of condensation and k_e of evaporation. Steady-state condition being assumed, the net change from gaseous water to the liquid or solid state can be calculated, if the H_2O concentration is known. Moreover, the concentration of liquid (plus solid) water can be derived from the continuity equation for water:

$$\frac{\partial [water]}{\partial t} = -(-k_c [H_2O] + k_e [water]) + \frac{\partial}{\partial z} [K_z M \frac{\partial [water]}{\partial z}] + v [water]$$

where v denotes the velocity of falling rain. The boundary condition for this equation is the amount of rainfall per year, set to 1000 mm/a.

It is now easy to calculate the amount of physically or chemically dissolved gases, if the pH-values for rain and clouds are given. The net reduction of gaseous components via preci-

precipitation is then proportional to the net reduction of water vapour from each layer of altitude.

$$\frac{\partial [X_{\text{gas}}] / \partial t}{\partial [H_2O] / \partial t} = \frac{[X_{\text{dissolved}}]}{[water]}$$

The proportionality factor is a function of pH-value, the liquid water concentration and the equilibrium constants. An extended example for the calculation is given by Gravenhorst et al. (1978).

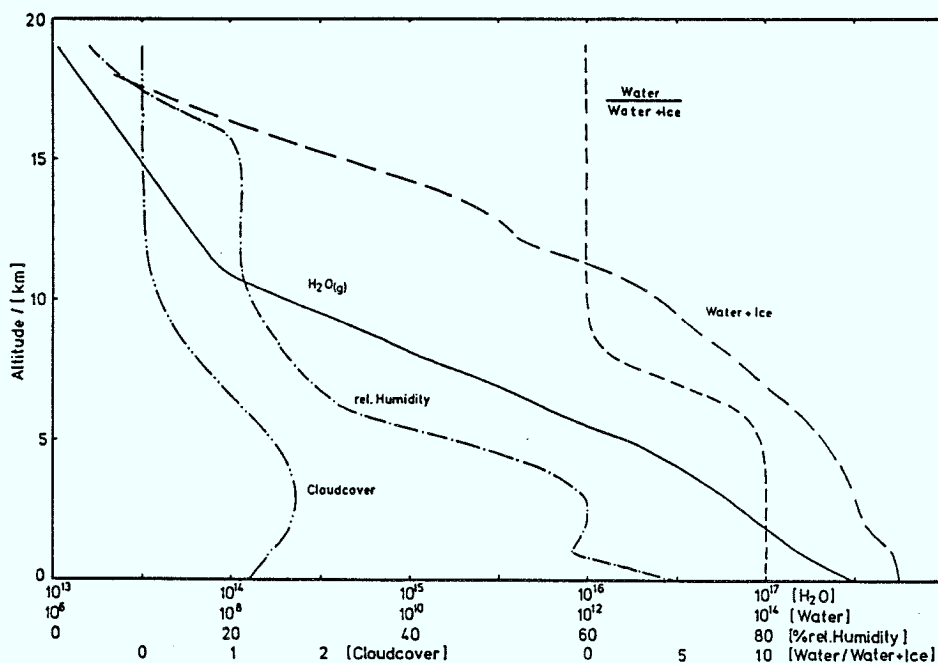


Figure 5: Altitudinal dependency of gaseous H_2O (—), of the total concentration of water + ice (---) and of the relative humidity (-.-). The cloud cover HKT (-.-.-) and the ratio of water to water + ice (x - x) are also plotted.

4.3 Averaging Procedures

The mass continuity equation for a one-dimensional model has to be integrated according to latitude and longitude. Besides this, it is necessary to integrate over the time step Δt :

$$\frac{1}{\Delta t} \int_0^{\Delta t} \frac{\partial C}{\partial t} dt = \frac{1}{\Delta t} \int_0^{\Delta t} (P - DC + \nabla \vec{j}) dt$$

Here, $\vec{j}$ stands for the mass flux $\vec{v} \cdot C$. As the influence of time varies with the nature of the reactions, we will discuss the averaging procedures for photochemistry, gas-phase chemistry, wash-out, and transport separately.

The photochemical reactions depend to a large extent on the pathlength of the photon flux through the atmosphere and therefore, on the solar zenith angle. To take this fact into account, a diurnal averaging procedure as well as seasonal averaging has to be carried out for the steady-state and long-term versions. The seasonal variations are omitted by using equinox conditions. As the absorption coefficients are independent of time (if we neglect variations with temperature), only the photon flux has to be averaged over time-steps, which are smaller than one day. For steady-state conditions and for time-steps bigger than 1 day, a diurnal average is attained from these fluxes:

$$\overline{F(Z)} = \int_0^{24h} F(t, Z) dt = \alpha(Z) \cdot F(Z)|_{\text{noon}}$$

where F_{noon} is the photonflux at noon. α is an averaging factor, calculated in a preceeding run of the diurnal variation version.

Concerning the gas-phase reactions, we use the same procedure as for the photochemical reactions. The diurnal variation version gives an averaging coefficient β_{ij} , which pays heed to the fact that the mean of a product is different to the product of the means:

$$\overline{k_{ij} \cdot \bar{C}_i \cdot \bar{C}_j} = \beta_{ij} \cdot k_{ij} \cdot \bar{C}_i \cdot \bar{C}_j$$

The altitudinal dependency of this averaging coefficient can be presented to a sufficient extent by a straight line:

$$\beta_{ij}(z) = a_{ij} + b_{ij}z$$

For the wet chemistry reactions, we have to consider that it is not raining or cloudy always and everywhere. We assume an altitude-dependent frequency of clouds and rain, taken from observations:

$$HKT(z) = 0.121 \exp(0.256z - 0.0436z^2)$$

This averaging factor enters the wet removal rate via the calculation of the actual amount of water present at the time of dissolution. The (time-averaged) water concentration, calculated according to the formula in chapter 4.2, has to be divided by the frequency of clouds and rain to get the actual amount.

As for the transport term, most averaging procedures are already included in the eddy-diffusion coefficient. For large time-steps a mean mass flux has to be used. This can be achieved by assuming a time-dependency of the mass flux resulting in an averaged value of

$$\bar{j} = j_{\infty} + (j_0 - j_{\infty}) \frac{1 - \exp(-\alpha \Delta t)}{\alpha \Delta t}$$

This is discussed in more detail in the following chapter.

5. Transport

5.1 Calculation of the Transport Term

Besides the variations of the concentration of a component of the atmosphere due to chemical reactions, the concentration is changed by transport. But it is impossible to calculate the transport term

$$\nabla(\vec{v} \cdot C)$$

in full detail, as the wind velocity $\vec{v}$ is highly dependent on location and time. Therefore a disturbance assumption is applied and the actual velocity is divided into a mean velocity $\vec{v}_0$ and its locally and temporally disturbed portion $\vec{v}'$

$$\vec{v} = \vec{v}_0 + \vec{v}'$$

The term $\vec{v}'$ contains all subgrid scale motions and the effect of these motions can be treated in analogy to molecular diffusion. Instead of the molecular diffusion constant a eddy-diffusion constant K_z is introduced, which has to be deduced from tracer observations. For a one-dimensional model only vertical transport is possible and the integral over the mean velocity $\vec{v}_0$ equals zero. The eddy-diffusion term is then expressed by

$$TT = \frac{\partial}{\partial z} \left[K_z M \frac{\partial}{\partial z} \left(\frac{C}{M} \right) \right]$$

For 1-D-models we consider the constant K_z a mere model parameter which is calculated by adjusting the calculations to a chemical tracer like N_2O , CH_4 or others (E.g.: Schmeltekopf et al., 1977, NAS, 1979, Massie and Hunten, 1981, Th. Janßen-Schmidt, 1982).

By using an eddy-diffusion assumption for the transport term, the mass continuity equation becomes a second-order differential equation in space. To solve this spatial differential equation system, we have to use an algorithm which results in a linear system. To achieve that no artificial sink or source is brought in by the mathematical treatment, we calculate the transport by considering the mass fluxes at an intermediate altitude between two neighbouring levels:

$$\overline{TT}_i = -\left. \frac{\partial \overline{J}}{\partial z} \right|_i = -\frac{\overline{J}_{i+1/2} - \overline{J}_{i-1/2}}{\Delta z}$$

with

$$\begin{aligned} \overline{J}_{i+1/2} &= -K_{i+1/2} M_{i+1/2} \left. \frac{\partial C}{\partial z M} \right|_{i+1/2} = \\ &= -\frac{K_{i+1} M_{i+1} + K_i M_i}{2} \frac{C_{i+1}/M_{i+1} - C_i/M_i}{\Delta z} \end{aligned}$$

and $\overline{J}_{i-1/2}$ correspondingly.

For the steady-state assumption, this leads to a set of equations

$$a_i \mu_{i-1} + (D_i M_i - b_i) \mu_i + c_i \mu_{i+1} = P_i \quad \text{with} \quad \mu_i = \frac{C_i}{M_i}$$

where D_i and P_i are the destruction frequency and the production rate for the specific component and a_i , b_i and c_i represent the transport term at an altitude $z = i \cdot \Delta z$. This linear equation set can easily be solved by a simplified Gauß elimination, provided that the boundary conditions are known (see also appendix A.1.1.).

The short-term, time-dependent version of the model depends only very slightly on transport. Therefore, it is sufficient to calculate the transport term at the beginning of a run and adjust it proportional to the concentration during the calculation. If we assume that the altitudinal trend of the concentration profile does not change during the course of the day, then it is possible to set $C(t) = C_0 \cdot f(t)$ with $df/dz = \text{const}$, and subsequently

$$TT(t) = TT_0 \cdot f(t) = TT_0 \cdot \frac{C(t)}{C_0}$$

In the long-term, time-dependent version of the model, we normally use time-steps which are in the order of the time of the mass exchange between two layers. So we cannot use the transport term calculated at time $t = t_0$ but we have to average this term over the period Δt . For the mass flux j we assume an exponential time dependency,

$$j(t) = j_{\infty} + (j_0 - j_{\infty}) e^{-\alpha t}$$

which leads to an averaged flux during Δt of

$$\bar{j} = j_{\infty} + (j_0 - j_{\infty}) \frac{1 - \exp(-\alpha \Delta t)}{\alpha \Delta t}$$

The parameter α is set equal for all components according to a Gaussian propagation:

$$\alpha = \frac{2K}{(\Delta z)^2}$$

The detailed description of the algorithm is given in appendix A.1.2. By using the long-term version of the model, it turned out, that the time step should not become larger than the time for mass transport over more than two layers, to exclude influences from layers not neighbouring the one for which the calculation takes place. So we are restricted to time steps smaller than three days.

5.2 Boundary Conditions

To solve the spatial, second-order differential equation two boundary conditions are necessary. At the upper boundary, we use constant mixing ratios. As these values are mostly unknown, we extend the calculations up to 99 km, and we underestimate the mixing ratios to achieve that the error is not larger than 100 %. Therefore the errors introduced by the estimation do not propagate down to 65 km, which is the altitude we consider our upper limit for the correct concentration profiles. This fact was tested in a series of runs under varying conditions.

At the lower boundary at ground level, two conditions are possible. We apply either constant mixing ratios as well or constant fluxes. For constant fluxes, especially if they include a deposition velocity, the spatial step of 1 km is too large to give correct mixing ratios in the troposphere, if a linear approximation, as in the case of the other altitudes, is used. To overcome this difficulty, either an auxiliary step at 0.3 km is introduced (which complicates the programming considerably) or a second-order Taylor approximation is assumed. In our model the second method is selected. We then obtain the following equation for the first level:

$$(3+2\Delta Z \frac{V_D}{K_0}) \cdot \frac{C_0}{M_0} - 4 \frac{C_1}{M_1} + \frac{C_2}{M_2} = 2\Delta Z \frac{j_{prod}}{K_0 M_0}$$

V_D is the deposition velocity and j_{prod} the production flux at ground level.

The boundary value of the eddy-diffusion coefficient can neither for the linear nor for the second-order approximation be chosen freely, as otherwise hidden sources or sinks are

introduced. In the case of the Taylor approximation, the $K_{z=0}$ value depends on $K_{z=1}$ and $K_{z=2}$:

$$K_{z=0} = \frac{K_1 M_1 \cdot K_2 M_2}{(2K_2 M_2 - K_1 M_1) \cdot M_0}$$

As for the time-dependent versions, there has to be an additional boundary condition for the first-order differential equation in time. For this we take the concentration profiles calculated in a preceding run of the steady-state version. Besides this initial boundary condition, there might be time-dependent sources of particular components, e.g. anthropogenic production at ground level or elsewhere. Therefore, the production terms at an altitude z_x have to be modified, if the time step Δt is in the order of the exchange rate with neighbouring layers. For large time-steps, other layers than z_x are influenced by the source, too. To take this into account, we assume an increase of concentration in the upward and downward directions according to a Gaussian propagation:

$$\Delta C = j_0 \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(z-z_x)^2}{2\sigma^2}\right) \Delta t$$

with

$$\sigma = \sqrt{\frac{K \Delta t}{2}}$$

This production term must be multiplied by 2 for $z_x = 0$ as there is no diffusion downwards. The assumptions included in this formula make it valid only for time steps not bigger than 1 week, so we are restricted to that.

6. Description of the Different Versions

At the moment no model can be applied for every purpose, so for different intentions, different types of models have to be used. Our basic model type is the steady-state version, but for long-time prognoses a time-dependent version is necessary with time-steps of the order of days or weeks. For diagnostic calculations, we make use of a diurnal variation model with variable time-steps between one second at sunset and sunrise and 15 minutes at noon and during the night. To achieve that the results of the different versions are comparable, the model is built in a modular technique using the same subprograms and program steps in all three types as far as possible. By doing so, it is also possible to use the same data sets in all versions, making the updating of the input parameters rather easy.

6.1 The Steady-State Version

As mentioned before, the steady-state version is the basic type of the model, providing the time-dependent programs with the starting values. So this version is described here in detail, whereas the next chapter describes only the modifications of the time-dependent model types. A flux diagram and the hierarchy of the subprograms are given in figure 6. After the FORTRAN-declarations, necessary for the program, the parameters are either read in from a disc or from cards or they are fixed via DATA-statements or assignment-statements. To avoid useless spending of computer time, the approximate profiles for all components are read in. These profiles are calculated in a preceding run with up to 1000 iterations starting with estimated profiles for each species. The influence of the number of iterations for the convergence of the procedure is shown in figure 7.

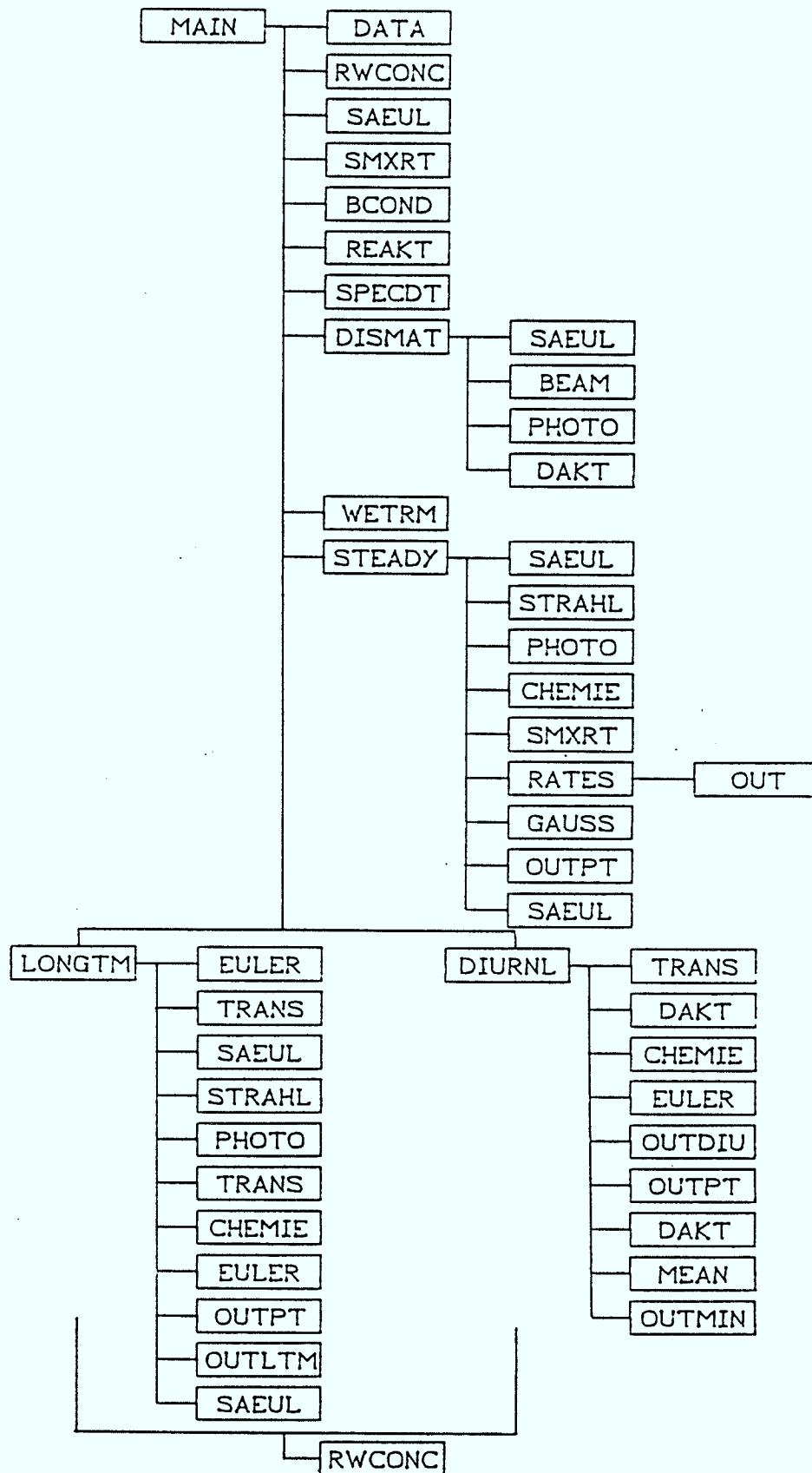
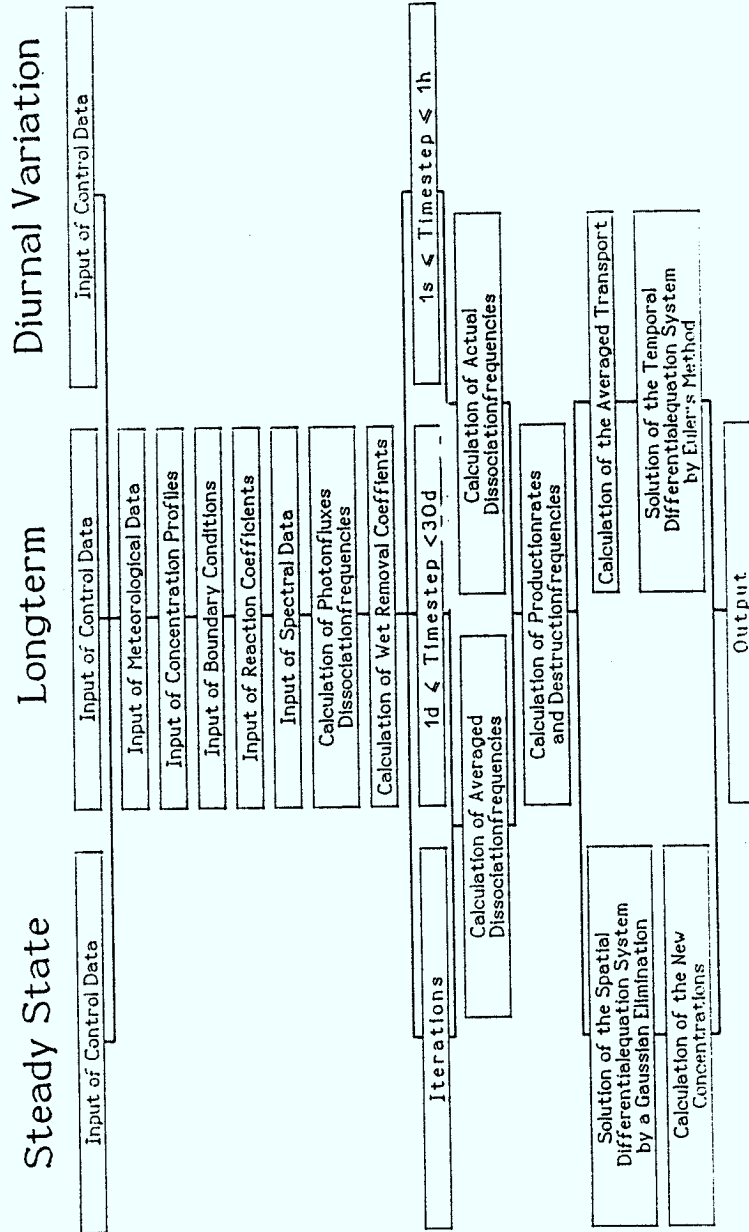


Figure 6: Flux diagram and hierarchy of subprograms.

Diagram of the 1D Model System



After the input of the concentration profiles, the boundary conditions are read in and the matrix elements for transport are calculated. Before the photodissociation coefficients can be calculated by the subprogram PHOTO, the solar flux and the absorption cross-sections have to be stored. The altitude dependence of the photon flux and of the column densities of the absorbing species are calculated in the subprograms FLUSS and SAEUL, respectively. The details of the calculations of the photo-dissociation are described in chapter 3 and in appendix A.1.3.

As the photo-dissociation rates vary with changing ozone- and NO_2 -concentration during the execution of the iterations, these coefficients have to be redetermined from time to time. As this procedure is the most time-consuming one, it is carried out only every 2^n iteration (with $n = 0, 1, 2, \dots$), once a year, or at the beginning of the short-term version. Figure 7 shows how the calculated concentrations converge with the number of calculations of the photo-dissociation rates.

The reaction constants for the homogeneous gas-phase reactions and the equilibrium constants or the coefficients of the heterogeneous reactions in water droplets are read in next, together with the coefficients of the averaging factors.

This input-block is used in all three versions of the model and then the program divides up into three branches.

The calculation of the production and destruction terms are carried out by the subprogram CHEMIE for all three models. For those components with life-times larger than the transport time, the mass continuity equation is solved separately. But for the constituents with fast exchanging rates, this is not possible as the transport term would then become negligible. So these components are grouped together and the whole

group, which now has slow production and destruction rates, is transported.

As the steady-state assumption:

$$\frac{\partial C}{\partial t} = 0$$

reduces the mass continuity equation to a second-order differential equation in space, this equation can be linearized to form a simple tensor equation for the mixing ratios. The tensor equation is solved by a Gaussian elimination. (For more details see chapter 5.1.) These mixing ratios are then transformed into concentrations and, by including the concentration ratios within the groups, the short-lived species are computed.

The last part of the program contains the output of the different values. After the last iteration, governed either by a convergence criterium or by a fixed number of iterations, the concentrations as well as the mixing ratios of all species are printed. Besides this print-out, it is possible to plot either the concentration profiles or the mixing ratios or both on a CALCOMP-Plotter using the subroutine HOEPRO. If it is of interest, the photo-dissociation rates can be printed and/or plotted, too. In special cases, during the last iteration the production rates and the destruction frequencies for all substances and every reaction are calculated and printed. The relative importance of the reactions for the overall production and destruction are plotted in semi-logarithmic graphs as shown in appendix A.2.

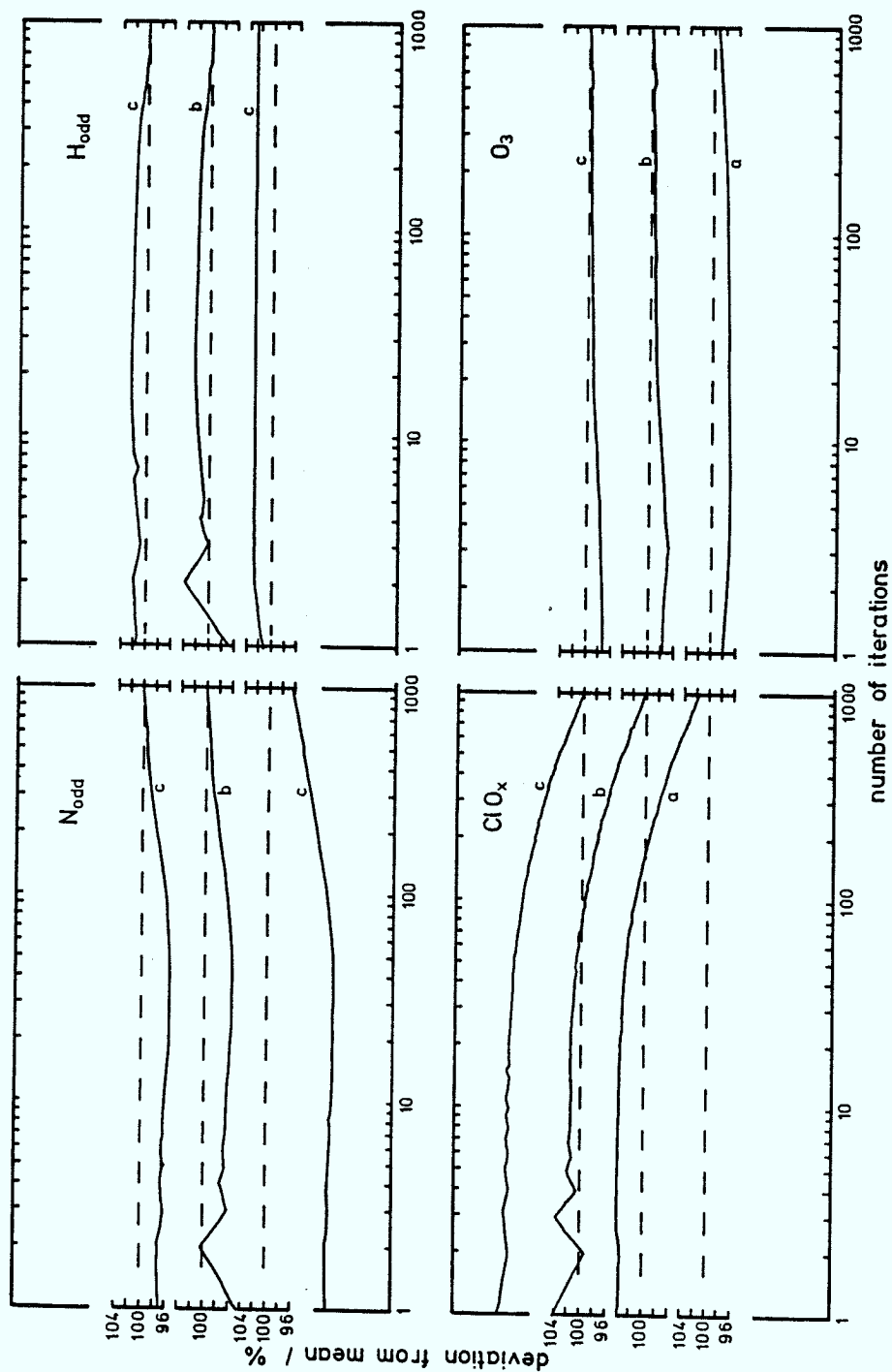


Figure 7a: The influence of the number of iterations on the calculations of the concentrations of different species or groups. The curves represent the calculations with a) no iteration, b) 3 iterations, and c) 5 iterations of the radical ratios within each group. The photon flux and the photodissociation frequencies are calculated for every 2^{th} iteration.

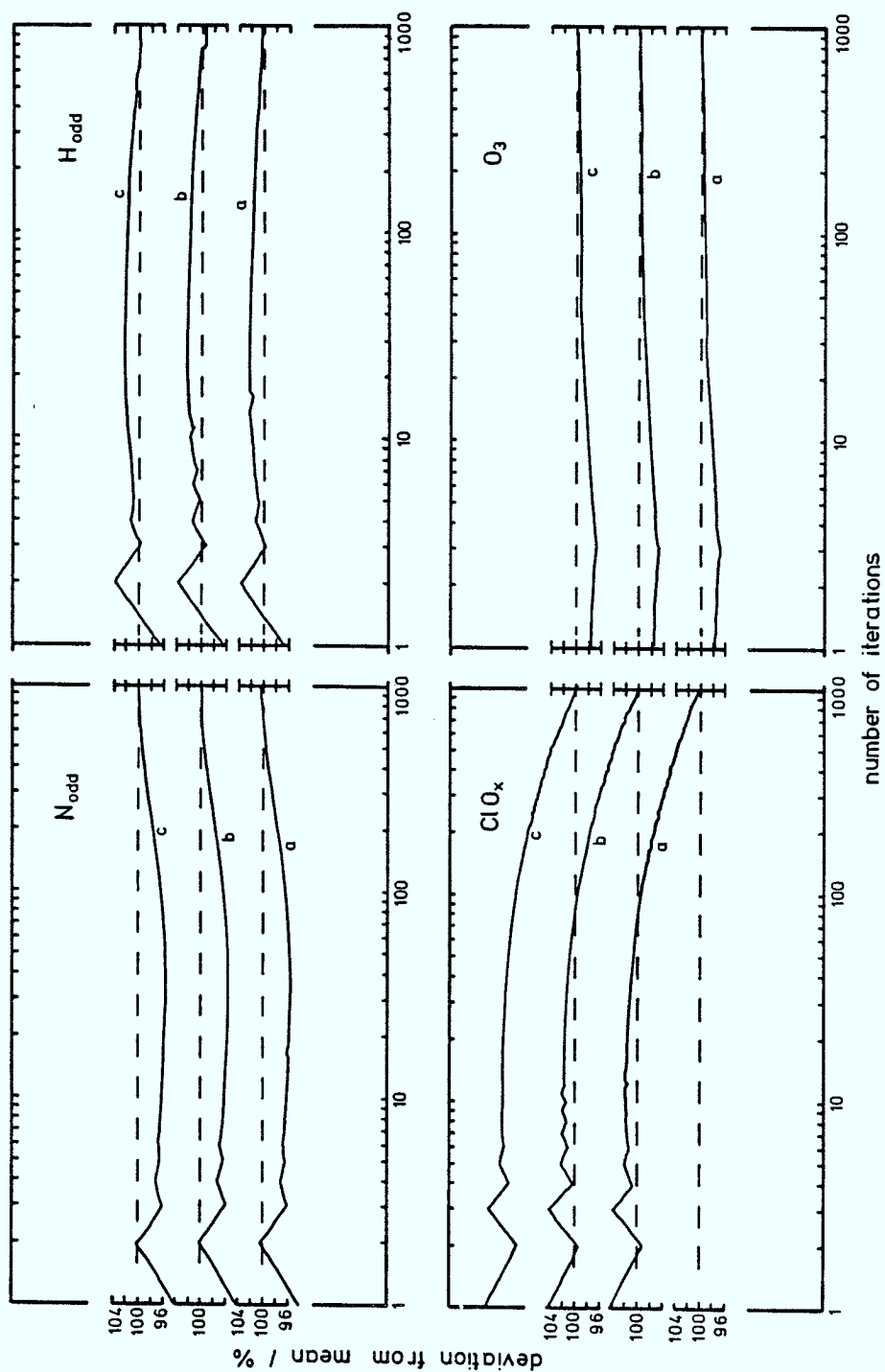


Figure 7b: The influence of the number of iterations and the number of calculations of the photodissociation frequencies for different species. The photon flux is calculated for a) every 2ⁿth, b) every 3ⁿth, and c) every 4ⁿth iteration.

6.2 The Time-Dependent Versions

For long-time prognosis a special version is used with time-steps larger than 1 day. The specific part of this program starts with the calculation of the averaged production and destruction terms as in the steady-state version.

To get a simplified, only time-dependent differential equation, the program uses a transport term, averaged over the time-step Δt . Then this transport term TT can be treated like a production term, resulting in a simple Euler's equation for the law of mass continuity:

$$\frac{\partial C}{\partial t} = (P + TT) - DC$$

This equation can be solved explicitly:

$$C_{t+\Delta t} = \frac{P+TT}{D} + \left(C_t - \frac{P+TT}{D} \right) e^{-D\Delta t}$$

The subprogram TRANS deduces the transport term and in the subprogram EULER the differential equation in time is solved.

For calculating the diurnal variations of the concentrations of the atmospheric components a short-term version is used. This version differs only slightly from the long-term one, but it uses variable time-steps between 0,01 sec at sunrise and sunset and 1.5 min at noon and during the night. On the other hand, and this is the main difference, the actual photo-dissociation and reaction rates are used. As the ozone column density varies only slightly during one single day, the photo-dissociation rates are calculated at certain zenith angles, and are then stored and the actual photo-dissociation rates are computed by interpolation.

To obtain a sufficiently accurate boundary condition in time, we start with the results of the steady-state version as in the long-term model. As the diurnally averaged photon flux corresponds approximately to that at about 10 o'clock, we start the calculation at that time. But we have to run the program for 14 days to achieve periodically stable conditions. This is due to the fact, that the state-state version do not distinguish between nighttime and daytime chemistry besides by the averaging factors.

The output of the time-dependent versions include print-outs of the concentration profiles at noon (as for the short-term version) and for the last time-step. Besides this, the mixing ratios are printed at specific time-steps and isolines, showing the time-dependence of the concentrations at certain altitudes, can be plotted.

For calculating the averaging coefficients of the gas-phase reactions and the photo-dissociation rates a subprogram MEAN can be activated. This subprogram averages the concentrations at every full hour during a whole day, as derived from the short-term version.

A.1. Algorithms

A.1.1. The Differential-Equation in Space

In order to achieve that no artificial source or sink of mass is introduced by the algorithm calculating the transport-term, we are considering the fluxes into and out of the layer $z - \Delta z/2 \leq z \leq z + \Delta z/2$, setting the flux out of one layer equal to the flux into the next layer.

The transport-term is given by

$$TT = -\frac{\partial}{\partial z}(j + v_s \cdot C)$$

with flux

$$j = -K_z \cdot M \cdot \frac{\partial}{\partial z} \frac{C}{M}$$

and v_s the sedimentation velocity of aerosols. With the abbreviations

$$\mu = \frac{C}{M} \quad Y = K_z \cdot M \quad V = v_s \cdot C = v_s \cdot M \cdot \mu$$

we assume

$$TT_i = -\frac{(j_i^u + V_i^u) - (j_i^b + V_i^b)}{\Delta z}$$

with the fluxes at the upper boundary of the layer

$$j_i^u = -\sqrt{Y_{i+1} \cdot Y_i} \frac{\mu_{i+1} - \mu_i}{\Delta z} \quad \text{and} \quad V_i^u = V_{i+1/2} \frac{M_{i+1}\mu_{i+1} + M_i\mu_i}{2}$$

and j_i^b and v_i^b at the bottom of the layer correspondingly. With these assumptions we obtain a linear equation system

$$TT_i = a_i \mu_{i-1} - b_i \mu_i + c_i \mu_{i+1}$$

The constants a, b, c, herein are defined as follows:

$$a_i = \frac{\sqrt{Y_i \cdot Y_{i-1}}}{(\Delta Z)^2} + v_{i-1/2} \frac{M_{i-1}}{2 \Delta Z}$$

$$b_i = \frac{\sqrt{Y_{i+1} \cdot Y_i} + \sqrt{Y_i \cdot Y_{i-1}}}{(\Delta Z)^2} + (v_{i+1/2} - v_{i-1/2}) \frac{M_i}{2 \Delta Z}$$

$$c_i = \frac{\sqrt{Y_{i+1} \cdot Y_i}}{(\Delta Z)^2} - v_{i+1/2} \frac{M_{i+1}}{2 \Delta Z}$$

For flux boundary conditions at the ground level, we assume a parabolic altitudinal dependency of the mixing ratio :

$$\frac{C}{M} = \mu = az^2 + bz + c$$

The flux j_0 at the ground level is given by the expressions

$$j_0 = j_{\text{Prod}} - v_D M_0 \mu_0$$

and

$$j_0 = -Y_0 \left. \frac{\partial \mu}{\partial z} \right|_0 = -Y_0 b$$

with j_{Prod} the production per area at the ground level and v_D the deposition velocity.

With μ_1 and μ_2 given, as is the normal case in our calculations, the lower boundary equation is

$$\mu_0 \left(3 + \frac{2\Delta z}{K_0} v_0\right) - 4\mu_1 + \mu_2 = \frac{2\Delta z}{K_0 M_0} j_{\text{Prod}}$$

Together with the upper boundary condition

$$\mu_u = \text{const}$$

the mass continuity equation for the steady-state case is linearized for all altitudes and can be solved by a simplified Gauß elimination.

In the case of the long-term version of the model, the fluxes into and out of the layer $z - \Delta z/2 \leq z \leq z + \Delta z/2$ have to be averaged over the time-step Δt . To calculate these averaged fluxes, we start with a 2nd order Taylor approximation for the mixing ratios.

Under the assumption that $K M \approx \text{constant}$ within the layer and under neglect of any chemistry involved, the mass continuity equation can be written as follows:

$$\begin{aligned} \frac{\partial C}{\partial t} &= \frac{\partial}{\partial z} \left[K M \frac{\partial \mu}{\partial z} \right] = K M \frac{\partial^2 \mu}{\partial z^2} \\ &= K M \frac{\mu_{i+1} + \mu_{i-1}}{(\Delta z)^2} - \frac{2 K M}{(\Delta z)^2} \mu_i = \\ &= \text{const} - \alpha C \quad \text{with} \quad \alpha = \frac{2K}{(\Delta z)^2} \end{aligned}$$

Solving this equation, the concentration C and the mass flux j are given by

$$\begin{aligned} C &= C_\infty + (C_0 - C_\infty) e^{-\alpha t} \\ j &= -K M \frac{\partial \mu}{\partial z} = j_\infty + (j_0 - j_\infty) e^{-\alpha t} \end{aligned}$$

From this time-dependency, the averaged flux can be derived:

$$\begin{aligned}\bar{j} &= \frac{1}{\Delta t} \int_0^{\Delta t} [j_{\infty} + (j_0 - j_{\infty}) e^{-\alpha t}] dt = \\ &= \frac{1}{\Delta t} [j_{\infty} t + \frac{1}{\alpha} (j_0 - j_{\infty}) e^{-\alpha t}] \Big|_0^{\Delta t} = \\ &= j_{\infty} + (j_0 - j_{\infty}) \frac{1 - e^{-\alpha \Delta t}}{\alpha \Delta t}\end{aligned}$$

The mass flux j_0 at the time t is calculated directly and j_{∞} is defined via the steady-state assumption

$$\frac{\partial C}{\partial t} = P - DC_{\infty} - \frac{\partial j_{\infty}}{\partial z} = 0$$

The values of C_{∞} and, correspondingly j_{∞} , are derived from a steady-state assumption with the actual boundary conditions at the time t . To minimize the computation time, j_{∞} is calculated only once every year and normalized to j_{∞}^{rel} . The actual flux j_{∞}^t is then given by

$$j_{\infty}^t = j_{\infty}^{rel} \cdot C_{Troposphere}^t$$

A.1.2. The Time-Dependent Differential Equation

For the transport term in the time-dependent models, we use the averaged mass flux described in appendix A.1.1.:

$$TT_i = -\frac{\overline{j_{i-1/2}} - \overline{j_{i+1/2}}}{\Delta z}$$

As this term is considered constant during time-step the Δt , the time-dependent differential equation of mass can be solved by the Euler's method:

$$\frac{\partial C}{\partial t} = (P + TT) - DC$$

The solution of this simple equation is:

$$C_{t+\Delta t} = \frac{P+TT}{D} + \left(C_t - \frac{P+TT}{D} \right) e^{-D\Delta t}$$

Actually this equation is only correct, if D does not equal 0. If, for a certain species, only production has to be considered, the solution of the Euler's equation is given by

$$C_{t+\Delta t} = C_t + (P + TT) \cdot \Delta t$$

Both cases are included in the subprogram EULER, which solves the time-dependent differential equation.

If, at a certain level z_x , there is an input of some constituent of the air, this will influence not only the concentration at level z_x . For time-steps longer than 1 day (the approximate diffusion time for a layer of thickness 1 km), the neighbouring layers are influenced, too. This can be taken into account by assuming a Gauss' function for the mixing ratio

$$\Delta u(z) = j_{\text{Prod}} \frac{\Delta t \cdot \text{factor}}{M(z)} e^{-\frac{(z-z_x)^2}{2\sigma^2}}$$

The half-width σ of this function is proportional to the time-step Δt and to the eddy-diffusion coefficient K_z , as shown above.

"factor" is the normalization factor, derived from

$$\int_0^{\infty} \Delta C \, dz = j_{\text{Prod}} \Delta t$$

This supplementary term is added to the concentrations calculated by means of the subprogram Euler.

A.1.3 Expression for the Photon-Flux

The flux diagram for the photons present at a level j in the atmosphere is outlined in figure 8. We consider two photon-fluxes, one downwards (F_d^j) and one upwards (F_u^j). These fluxes are given by

$$F_d^j = F_d^{j+1} \cdot e^{-\Delta\tau} \cdot e^{-\Delta\tau_R} + \sum_{i=1}^{\infty} {}^iH_d + \sum_{i=1}^{\infty} {}^iI_d - Z^j$$

and

$$F_u^j = F_u^{j-1} \cdot e^{-\Delta\tau} \cdot e^{-\Delta\tau_R} + \sum_{i=1}^{\infty} {}^iH_u + \sum_{i=1}^{\infty} {}^iI_u + Z^j$$

Here $\Delta\tau$ and $\Delta\tau_R$ are the optical densities for pure absorption and for Rayleigh scattering within the layer considered. ${}^iH_d$ and ${}^iH_u$ are the fractions of the flux F_u scattered into the direction of the flux and against it. Z^j gives the flux reflected at the cloud's surface at the level j :

$$Z^j = F_d^{j+1} \cdot e^{-\Delta\tau} \cdot e^{-\Delta\tau_R} \cdot A_{\text{cloud}}^j$$

A_{cloud}^j consists of the cloud albedo multiplied by the averaged cloud cover at the level j .

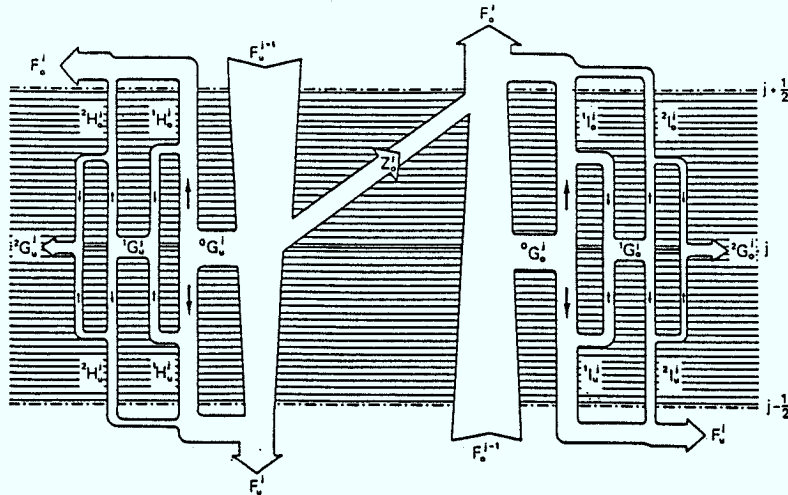


Figure 8: The flux diagram for the solar radiation within the level j . F_u and F_d are the fluxes, G_u and G_d the amount of the scattered photons and H_u and H_d the fluxes of the scattered photons. Z represents the portion of the downward flux reflected at the cloud's surface.

The scattered photon-fluxes are presented by the terms $\sum H$ and $\sum I$. The amount ${}^i G_d$ of the photons scattered from the downward flux is given by

$${}^i G_d = {}^{i-1} G_d e^{-\Delta\tau} (1 - e^{-\Delta\tau_R}) = F_d^{j+1} e^{-\Delta\tau} (1 - e^{-\Delta\tau_R})^{i+1}$$

with

$${}^0 G_d = F_d^{j+1} e^{-\Delta\tau} (1 - e^{-\Delta\tau_R})$$

and similarly for the upward flux.

The total amount of photons present at a certain level j is then:

$$F_{\text{tot}}^j = F_d^j + F_u^j + \sum_{i=0}^{\infty} {}^i G_d + \sum_{i=0}^{\infty} {}^i G_u$$

The sum $\sum {}^i G$ in this equation is a geometric series, the result of which is known:

$$\sum_{i=0}^{\infty} {}^i G_d = F_d^{j+1} e^{-\Delta\tau} \sum_{i=0}^{\infty} (1 - e^{-\Delta\tau_R})^{i+1} = F_d^{j+1} \frac{1 - e^{-\Delta\tau_R}}{1 - e^{-\Delta\tau}(1 - e^{-\Delta\tau_R})}$$

If we now assume with Isaksen et al. (1976) that half of the scattered photons are going backwards and half forwards, the sum $\sum H$ in flux F can be expressed in the same way:

$${}^i H_d = {}^i H_u = \frac{1}{2} e^{-\Delta\tau} e^{-\Delta\tau_R} {}^{i-1} G_d$$

$$\sum_{i=1}^{\infty} {}^i H_d = \sum_{i=1}^{\infty} {}^i H_u = \frac{1}{2} e^{-\Delta\tau} e^{-\Delta\tau_R} F_d^{j+1} \sum_{i=0}^{\infty} {}^i G_d = F_d^{j+1} \cdot \text{factor}$$

The factor is a function of the optical densities for pure absorption and for Rayleigh scattering:

$$\text{factor} = \frac{e^{-2\Delta\tau} e^{-\Delta\tau_R} (1 - e^{-\Delta\tau_R})}{2(1 - e^{-\Delta\tau}(1 - e^{-\Delta\tau_R}))}$$

The respective formulas are valid for the upward flux and with these assumptions the total amount of photons can be computed, provided the term I_u in the equation for F_d^j is known. To avoid time-consuming iterations, the flux F_u^{j-1} is estimated by the assumption, that below the layer j there is only one more layer:

$$(F_u^{j-1})_{\text{estimated}} = F_d^j \frac{(2A_g + (1-2A_g)(1-e^{-\tau_k^*}))e^{-2\tau^*}e^{-\tau_k^*}}{2-e^{-\tau^*}(2+A_g e^{-\tau^*}e^{-\tau_k^*})(1-e^{-\tau_k^*})}$$

As $\sum I_d$ is a rather small fraction of the flux F_d^j , the error made by the estimation does not propagate too much into the algorithm, whereas the advantage of saving computer-time is essential.

The calculation is done first downwards for F_d^j with an estimated (F_u^j) and then upwards for F_u^j and F_{tot} . The comparison of the results with the calculations of Luther and Gelinas (1975) are presented in figure 3.

A.2. List of Reaction Coefficients and Diagrams of Reaction Rates

The reaction coefficients used in our model are mainly the latest recommended data. At present we use those published by DeMore et al. (1985). They are listed in table 2a for bimolecular reactions and in table 2b for threebody reactions. The formulas for the time and pressure dependencies applied to calculate the actual rate coefficients are

$$k = k^0 \cdot e^{-T_0/T}$$

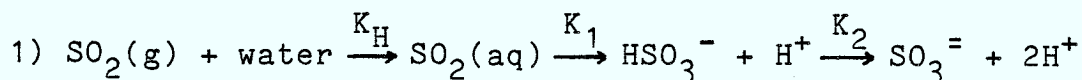
and

$$k = \frac{k^0 \cdot M}{1 + k^0 \cdot M/k^\infty} \cdot 0.6^{[1 + (\lg(k^0 \cdot M/k^\infty))^2]^{-1}}$$

with

$$k' = k_i^{\infty} \cdot \left(\frac{T}{300}\right)^n$$

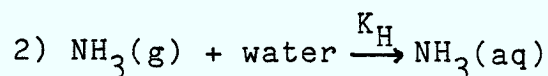
Regarding the wet chemistry, we are only interested in it as a sink for atmospheric compounds and we therefore only calculate the sum of dissolved components from Henry's law and subsequent equilibria. Explicitly the reactions considered are:



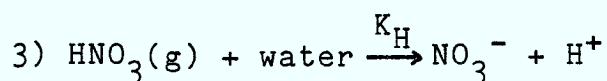
$$\text{with } K_H = 2.13 \text{ E-26 } \exp(3145/T)$$

$$K_1 = 1.90 \text{ E-5 } \exp(2022/T)$$

$$K_2 = 2.40 \text{ E-10 } \exp(1671/T)$$



$$K_H = 1$$



$$K_H = 5.40 \text{ E-28 } \exp(8650/T)$$



$$K_H = 3.30 \text{ E-26 } \exp(2268/T)$$

For HCl we use the same wet chemistry life-time as for HNO_3 and for H_2O_2 the same as for water.

By use of the subprogram RATES (see appendix A.4.), it is possible to indicate the relative importance of each reaction for the total production or destruction rate of a compound of the atmosphere. In figure 9, an example of the altitudinal dependencies of all reactions contributing more than 0.1 % to the overall reaction rate is plotted. The symbols used for the reactions are those of Hampson and Garvin (1976). The meaning of the symbols is explained in table 3.

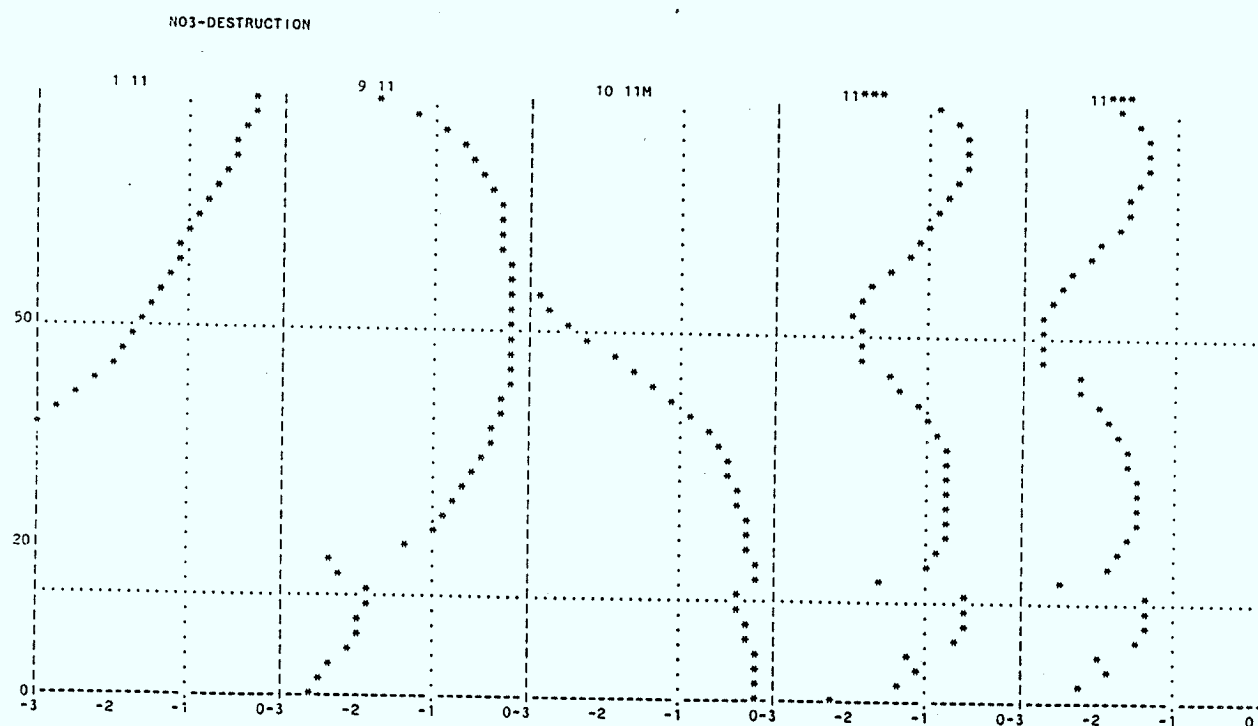


Figure 9: Example of a plot of the relative importance of the separate reactions for the overall production or destruction rate of a compound of the air. The symbols for the reactions are explained in table 3.

Table 2a: Bimolecular reactions and factors for the reaction constants used in the one-dimensional model system. The reaction constant is $k = A \exp(-T_a/T)$. The values are the recommended data of DeMore et al. (1985) if not otherwise indicated.

Reaction	A	T _a
O + O ₃ → O ₂ + O ₂	8.00E-12	2060
O + NO ₂ → O ₂ + NO	9.30E-12	
O + NO ₃ → O ₂ + NO ₂	1.00E-11	
O + OH → O ₂ + H	2.20E-11	-117
O + HO ₂ → O ₂ + OH	3.00E-11	-200
O + H ₂ → H + OH	8.80E-12	4200 a
O + H ₂ O → OH + OH	1.10E-10	9240 b
O + H ₂ O ₂ → OH + HO ₂	1.40E-12	2000
O + HS → H + SO	1.60E-10	
O + H ₂ S → OH + HS	1.00E-11	1810
O + ClO → O ₂ + Cl	4.70E-11	50
O + HCl → OH + Cl	1.00E-11	3340
O + HOCl → OH + ClO	1.00E-11	2200
O + CHO → OH + CO	2.10E-10	b
O + CH ₂ O → OH + CHO	3.00E-11	1550
O + CH ₃ → H + CH ₂ O	1.10E-10	
O + CH ₄ → OH + CH ₃	3.50E-11	4550 b
O + C ₂ H ₂ → CO + CH ₂ O	2.90E-11	1600
O + CH ₃ Cl → ClO + CH ₃	2.20E-11	3450 b
O + COS → SO + CO	2.10E-11	2200
O + HNO ₃ → NO ₂ + OH + O ₂	7.00E-11	3370
O + ClNO ₃ → NO ₂ + Cl + O ₂	3.00E-12	808
O(1D) + O ₂ → O + O ₂	3.20E-11	-67
O(1D) + O ₃ → O ₂ + O ₂	1.20E-10	
O(1D) + O ₃ → O + O + O ₂	1.20E-10	
O(1D) + N ₂ → O + N ₂	1.80E-11	-107
O(1D) + N ₂ O → O ₂ + N ₂	4.90E-11	
O(1D) + H ₂ O → NO + OH	6.70E-11	
O(1D) + NH ₃ → NO ₂ + OH + H ₂	2.50E-10	
O(1D) + H ₂ → H + OH	1.00E-10	
O(1D) + H ₂ O → OH + OH	2.20E-10	
O(1D) + H ₂ O ₂ → OH + HO ₂	2.80E-10	c
O(1D) + HCl → OH + Cl	1.50E-10	
O(1D) + CO ₂ → O + CO ₂	7.40E-11	-117
O(1D) + CH ₄ → H ₂ + CH ₂ O	1.40E-11	
O(1D) + CH ₄ → OH + CH ₃	1.40E-10	
O(1D) + C ₂ H ₂ → CH ₂ O + CH ₂ O	3.00E-10	
O(1D) + C ₂ H ₆ → CH ₂ O + CH ₂ O	3.20E-10	c
O(1D) + C ₃ H ₈ → 3 CH ₂ O	1.00E-10	c
O(1D) + F ₁₂ → 2 ClO	1.40E-10	
O(1D) + F ₁₁ → 3 ClO	2.30E-10	
O(1D) + CCl ₄ → 4 ClO + CO	3.30E-10	
O(1D) + COS → SO ₂ + CO ₂	1.50E-10	c
O ₂ + N → O + NO	4.40E-12	3220
O ₂ + SO → O + SO ₂	2.40E-13	2370
O ₂ + CHO → HO ₂ + CO	3.50E-12	-140
O ₂ + CH ₃ → OH + CH ₂ O	3.00E-16	
O ₂ + CH ₃ O → HO ₂ + CH ₂ O	8.40E-14	1200
O ₃ + N → O ₂ + NO	1.00E-15	
O ₃ + NO → O ₂ + NO ₂	1.80E-12	1370
O ₃ + NO ₂ → O ₂ + NO ₃	1.20E-13	2450
O ₃ + H → O ₂ + OH	1.40E-10	470
O ₃ + OH → O ₂ + HO ₂	1.60E-12	940
O ₃ + HO ₂ → 2O ₂ + OH	1.40E-14	580
O ₃ + SO → O ₂ + SO ₂	3.60E-12	1100
O ₃ + HS → SO ₂	3.20E-12	
O ₃ + Cl → O ₂ + ClO	2.80E-11	257
O ₃ + CH ₃ → OH + CH ₂ O	5.40E-12	220
N + NO → O + N ₂	3.40E-11	
N + NO ₂ → O + N ₂ O	3.00E-12	
N + OH → NO + H	4.50E-11	-60 d
NO + NO ₃ → NO ₂ + NO ₂	1.30E-11	-250
NO + HO ₂ → NO ₂ + OH	3.70E-12	-240

Table 2a continued

NO	+ ClO	→	NO ₂	+ Cl	6.20E-12	-294
NO	+ CH ₃ O ₂	→	NO ₂	+ CH ₃ O	4.20E-12	-180
NO ₂	+ H	→	NO	+ OH	4.80E-10	400 b
NO ₂	+ HO ₂	→	HNO ₂	+ O ₂	3.00E-15	e
NO ₂	+ CH ₃ O	→	HNO ₂	+ CH ₂ O	6.70E-15	b
N ₂ O ₅		→	NO ₂	+ NO ₃	* 1	
N ₂ O ₅	+ H ₂ O	→	HNO ₃	+ HNO ₃	1.00E-21	
NH ₃	+ OH	→	H ₂ O	+ NO ₂ + H ₂	3.50E-12	925
H	+ HO ₂	→	O ₂	+ H ₂	2.20E-11	
H	+ HO ₂	→	OH	+ OH	5.20E-11	
H	+ H ₂ O ₂	→	HO ₂	+ H ₂	2.50E-12	1400 b
H	+ H ₂ O ₂	→	OH	+ H ₂ O	2.70E-12	1400 b
H	+ HCl	→	H ₂	+ Cl	1.80E-11	1750 f
OH	+ OH	→	O	+ H ₂ O	4.20E-12	242
OH	+ HO ₂	→	O ₂	+ H ₂ O	1.70E-11	-416
OH	+ H ₂	→	H	+ H ₂ O	6.10E-12	2030
OH	+ H ₂ O ₂	→	HO ₂	+ H ₂ O	3.10E-12	187
OH	+ HNO ₂	→	NO ₂	+ H ₂ O	6.60E-12	b
OH	+ HNO ₃	→	NO ₃	+ H ₂ O	7.20E-15	-785
OH	+ H ₂ S	→	H ₂ O	+ HS	5.90E-12	65
OH	+ ClO	→	HO ₂	+ Cl	1.00E-11	-120
OH	+ HCl	→	H ₂ O	+ Cl	2.60E-12	350
OH	+ HOCl	→	H ₂ O	+ ClO	3.00E-12	150
OH	+ CO	→	H	+ CO ₂	1.50E-13	
OH	+ CH ₂ O	→	H ₂ O	+ CHO	1.00E-11	
OH	+ CH ₄	→	H ₂ O	+ CH ₃	2.36E-12	1710
OH	+ C ₂ H ₂	→	H ₂ O	+ 2 CH ₂ O	2.00E-12	250 g
OH	+ C ₂ H ₆	→	H ₂ O	+ 2 CH ₂ O	1.10E-11	1090
OH	+ C ₃ H ₈	→	H ₂ O	+ 3 CH ₂ O	1.60E-11	800
OH	+ F ₂	→	2 ClO	+ H ₂ O	1.00E-12	3650
OH	+ F ₂	→	3 ClO	+ H ₂ O	1.00E-12	3650
OH	+ CCl ₄	→	2 ClO	+ CO + 2 HCl	4.00E-15	b
OH	+ CH ₃ Cl	→	H ₂ O	+ Cl + ...	1.80E-12	1112
OH	+ CH ₃ CCl ₃	→	H ₂ O	+ 3 Cl + CH ₂ O	5.40E-12	1820
OH	+ CHCl ₃	→	H ₂ O	+ 3 Cl + CO	3.30E-12	1034
OH	+ COS	→	HS	+ CO ₂	3.90E-13	1780
OH	+ HNO ₄	→	O ₂	+ NO ₂ + H ₂ O	5.90E-13	-650 h
OH	+ ClONO ₂	→	HNO ₃	+ ClO	1.20E-12	333
HO ₂	+ HO ₂	→	O ₂	+ H ₂ O ₂	2.30E-13	-590
HO ₂	+ SO ₂	→	OH	+ H ₂ SO ₄	1.00E-18	
HO ₂	+ HS	→	H ₂ O	+ SO	5.00E-12	
HO ₂	+ HS	→	O ₂	+ H ₂ S	3.00E-11	
HO ₂	+ Cl	→	O ₂	+ HCl	1.80E-11	-170
HO ₂	+ Cl	→	OH	+ ClO	4.10E-11	450
HO ₂	+ ClO	→	HOCl	+ O ₂	4.60E-13	-710
HO ₂	+ CH ₂ O	→	H ₂ O ₂	+ CHO	4.50E-14	
HO ₂	+ CH ₃ O ₂	→	O ₂	+ OH + CH ₃ O	7.70E-14	-1300
H ₂	+ Cl	→	H	+ HCl	3.70E-11	2300
H ₂ O ₂	+ HS	→	HO ₂	+ H ₂ S	5.00E-15	
H ₂ O ₂	+ Cl	→	HO ₂	+ HCl	1.10E-11	980
HNO ₃	+ Cl	→	NO ₃	+ HCl	1.70E-14	
SO ₂	+ CH ₃ O ₂	→	CH ₃ O	+ H ₂ SO ₄	5.00E-17	
Cl	+ HOCl	→	OH	+ Cl ₂	3.00E-12	130
Cl	+ CH ₂ O	→	HCl	+ CHO	8.20E-11	34
Cl	+ CH ₄	→	HCl	+ CH ₃	9.60E-12	1350
Cl	+ C ₂ H ₂	→	HCl	+ 2 CH ₂ O	1.00E-12	
Cl	+ C ₂ H ₆	→	HCl	+ 2 CH ₂ O	7.70E-11	90
Cl	+ C ₃ H ₈	→	HCl	+ 3 CH ₂ O	1.40E-10	-40
Cl	+ CH ₃ Cl	→	HCl	+ HCl + CO	3.40E-11	1260
Cl	+ HNO ₄	→	O ₂	+ NO ₂ + HCl	3.00E-12	300
Cl	+ ClONO ₂	→	O	+ NO ₂ + Cl ₂	6.80E-12	-160
ClO	+ ClO	→	O ₂	+ Cl ₂	5.00E-13	1238
CO	+ CH ₃ O	→	CO ₂	+ CH ₃	4.00E-17	b
CH ₃ O ₂	+ CH ₃ O ₂	→	CH ₃ O	+ CH ₃ O + O ₂	1.60E-13	-220
HNO ₄		→	NO ₂	+ HO ₂	* 2	

* 1: Equilibrium constant $K = 1.52 \text{ E-}27 \exp(11153/T)$

* 2: Equilibrium constant $K = 2.33 \text{ E-}27 \exp(10870/T)$

a) Dubinsky and McKenney (1975), b) Humpson and Garvin (1978), c) Schofield (1978), d) Howard and Smith (1981), e) Howard (1977), f) Kita and Stedman (1982), g) Schmith and Zellner (1973), h) Schmith et al. (1984).

Table 2b: Threebody reactions and factors for the reaction constants used in the one-dimensional model system. The reaction constant is according to Troe (1983)

$$k = \frac{k_0 (300/T)^n [M]}{1+y} 0.6 (1 + (\lg y)^2)^{-1}$$

with

$$y = \frac{k_0 (300/T)^n [M]}{k (300/T)^m}$$

The values are the recommended data of DeMore et al. (1985), if not otherwise indicated.

Reaction			k_0	n	k	m
O	+ O	-M→ O ₂	1.65E-31	-2.6	0.00E+00	0.0 a
O	+ O ₂	-M→ O ₃	6.00E-34	2.3	0.00E+00	0.0
O	+ N	-M→ NO	1.04E-32	0.5	0.00E+00	0.0 b
O	+ NO	-M→ NO ₂	9.00E-32	1.5	3.00E-11	0.0
O	+ NO ₂	-M→ NO ₃	9.00E-32	2.0	2.20E-11	0.0
O	+ SO	-M→ SO ₂	1.90E-31	0.0	0.00E+00	0.0 b
O	+ SO ₂	-M→ ...H ₂ SO ₄	7.90E-34	-4.3	0.00E+00	0.0
O(1D)	+ N ₂	-M→ N ₂ O	3.50E-37	0.6	0.00E+00	0.0
O ₂	+ H	-M→ HO ₂	5.50E-32	1.6	7.50E-11	0.0
O ₂	+ CH ₃	-M→ CH ₃ O ₂	4.50E-31	2.0	1.80E-12	1.7
NO	+ OH	-M→ HNO ₂	7.00E-31	2.6	1.50E-11	0.5
NO ₂	+ OH	-M→ HNO ₃	2.60E-30	3.2	2.40E-11	1.3
NO ₂	+ HO ₂	-M→ HNO ₄	2.00E-31	2.7	4.20E-12	2.0
NO ₂	+ NO ₃	-M→ N ₂ O ₅	2.20E-30	4.3	1.50E-12	0.5
NO ₂	+ ClO	-M→ ClNO ₃	1.80E-31	3.4	1.50E-11	1.9
H	+ H	-M→ H ₂	8.30E-33	0.0	0.00E+00	0.0 b
OH	+ OH	-M→ H ₂ O ₂	6.90E-31	0.8	1.00E-11	1.0
OH	+ HO ₂	-M→ O ₂ +H ₂ O	1.60E-30	0.0	0.00E+00	0.0
OH	+ SO ₂	-M→ ...H ₂ SO ₄	3.00E-31	3.3	1.50E-12	0.0
OH	+ CO	-M→ H + CO ₂	3.50E-33	0.0	0.00E+00	0.0
OH	+ HNO ₃	-M→ NO ₃ +H ₂ O	2.13E-32	2.8	4.98E-14	5.6
HO ₂	+ HO ₂	-M→ O ₂ +H ₂ O ₂	4.60E-32	4.6	0.00E+00	0.0
Cl	+ Cl	-M→ Cl ₂	1.10E-32	3.8	0.00E+00	0.0 b

a) Slanger and Black (1976)

b) Hampson and Garvin (1978)

Table 3: List of the symbols marking the reactions in figure 9. Each reaction abbreviation consists of two numbers for the reaction partners. These numbers are:

1 $O(^3P)$	18 H	34 H_2SO_4	51 CH_3O_2
2 $O(^1D)$	19 OH	35 Cl	56 CH_4
4 O_2	20 HO_2	36 ClO	57 C_2H_2
7 O_3	21 H_2	39 HCl	58 C_2H_6
8 N	22 H_2O	40 HOCl	60 C_3H_8
9 NO	23 H_2O_2	44 Cl_2	61 CF_2Cl_2
10 NO_2	25 HNO_2	45 CO	62 $CFC1_3$
11 NO_3	26 HNO_3	46 CO_2	63 CCl_4
12 N_2	27 SO	47 CHO	64 CH_3Cl
13 N_2O	28 SO_2	48 CH_2O	68 COS
14 N_2O_5	31 HS	49 CH_3	69 HNO_4
17 NH_3	32 H_2S	50 CH_3O	70 $ClNO_3$

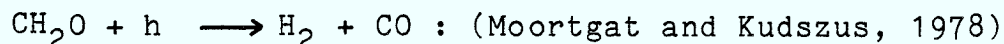
A.3. Absorption Cross-Sections, Quantum Yields, and Dissociation Energies

In this section we present the absorption spectra of the species being photodissociated in the atmosphere. The cross-sections are plotted in fig. 10, and the photo-dissociation reactions are listed in table 4. As several reactions possess threshold energies, the quantum yield has to be taken into account. For the calculation of the quantum yields, we apply the formula (a Fermi function)

$$\phi^{\lambda} = \frac{1}{\exp\left(\frac{\lambda - \lambda_0}{\Delta\lambda}\right) + 1}$$

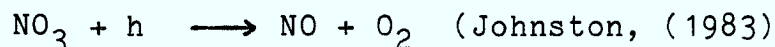
The coefficient λ_0 of this formula is temperature and/or pressure dependent, approximated by a linear dependency. The parameters of λ_0 are listed in table 5.

The quantum yields of CH_2O and NO_3 are a little bit more complicated and we use the following formulas for the respective reactions:



$$\phi = \frac{1}{\exp(x_1) + 1} - \frac{0.83}{\exp(x_2) + 1}$$

$$X_1 = \frac{\lambda - (342 + 4.7/p)}{7.3 + 1.57/p} \quad X_2 = \frac{\lambda - 3229}{4.7}$$



$$\phi = \frac{1}{\exp(x_1) + 1} - \frac{1}{\exp(x_2) + 1}$$

$$X_1 = \frac{\lambda - 608}{9.1} \quad X_2 = \frac{\lambda - 597}{13}$$

Table 4: Photo-dissociation reactions and reference list of absorption spectra.

Reaction			Spectrum	Wavelength Region	
O_2	$+ h\nu \rightarrow O$	$+ O$	Ackerman /1971/	1846.5	to 2424.5
O_3	$+ h\nu \rightarrow O(1D)$	$+ O_2$	Ackerman /1971/	1846.5	to 7300.0
O_3	$+ h\nu \rightarrow O$	$+ O_2$	Fairchild + Lee /1978/	2516.0	to 2920.0
NO	$+ h\nu \rightarrow O$	$+ N$	Ackerman /1971/	1846.5	to 7300.0
NO_2	$+ h\nu \rightarrow O$	$+ NO$	Fairchild + Lee /1978/	2516.0	to 2920.0
NO_3	$+ h\nu \rightarrow O$	$+ NO_2$	Nicolet /1979/	1846.5	to 1846.5
NO_3	$+ h\nu \rightarrow O_2$	$+ NO$	Bass et al. /1976/	1846.5	to 4050.0
N_2O	$+ h\nu \rightarrow O(1D)$	$+ N_2$	NASA-Report /1977/	4050.0	to 7000.0
N_2O_5	$+ h\nu \rightarrow O$	$+ 2 NO_2$	NASA-Report /1977/	4050.0	to 7000.0
NH_3	$+ h\nu \rightarrow NO_2$	$+ H + H_2O$	Nicolet + Peetermans /1972/	1846.5	to 2484.5
H_2O	$+ h\nu \rightarrow H$	$+ OH$	Johnston + Selwyn /1975/	2116.5	to 3005.0
H_2O_2	$+ h\nu \rightarrow OH$	$+ OH$	NASA-Report /1977/	2051.5	to 3800.0
COS	$+ h\nu \rightarrow CO$	$+ SO_2$	Thompson et al. /1963/	1846.5	to 2339.5
HNO_3	$+ h\nu \rightarrow NO_2$	$+ OH$	Hochanadel et al. /1972/	1846.5	to 1998.2
SO_2	$+ h\nu \rightarrow O$	$+ SO$	Lin et al. /1978/	1846.5	to 3500.0
ClO	$+ h\nu \rightarrow O$	$+ Cl$	NASA /1979/	1846.5	to 2234.5
HCl	$+ h\nu \rightarrow H$	$+ Cl$	Breckenridge + Taube /1970/	2234.5	to 2581.5
CO_2	$+ h\nu \rightarrow O$	$+ CO$	Biaume /1973/	1846.5	to 3450.0
CH_2O	$+ h\nu \rightarrow H_2$	$+ CO$	Thompson et al. /1963/	1846.5	to 3300.0
CH_2O	$+ h\nu \rightarrow H$	$+ CHO$	Kelly et al. /1976/	3350.0	to 4000.0
CF_2Cl_2	$+ h\nu \rightarrow 2 Cl$		Johnston et al. /1969/	2260.0	to 2721.5
$CFCI_3$	$+ h\nu \rightarrow 3 Cl$		Rigaud et al. /1977/	2759.0	to 3200.0
CCl_4	$+ h\nu \rightarrow 4 Cl$		Inn /1975/	1846.5	to 2186.0
CH_3Cl	$+ h\nu \rightarrow Cl$	$+ CH_3$	Shemansky /1972/	1846.5	to 3005.0
$ClNO_3$	$+ h\nu \rightarrow NO_2$	$+ ClO$	Moortgat /1979/	2234.5	to 3600.0
HO_2	$+ h\nu \rightarrow O$	$+ OH$	Moortgat /1979/	2234.5	to 3600.0
$HOC1$	$+ h\nu \rightarrow OH$	$+ Cl$	Hubrich et al. /1977/	1846.5	to 2395.5
$HOC1$	$+ h\nu \rightarrow O$	$+ HCl$	Hubrich et al. /1977/	1846.5	to 2759.0
Cl_2	$+ h\nu \rightarrow Cl$	$+ Cl$	Rowland + Molina /1975/	1846.5	to 2260.0
CH_3O_2	$+ h\nu \rightarrow O$	$+ CH_3O$	Hubrich et al. /1977/	1846.5	to 2367.0
HNO_2	$+ h\nu \rightarrow NO_2$	$+ H$	NASA-Data Eval. /1979/	1846.5	to 4500.0
HNO_2	$+ h\nu \rightarrow NO$	$+ OH$	Hochanadel et al. /1972/	1846.5	to 2685.0
HNO_4	$+ h\nu \rightarrow NO_2$	$+ HO_2$	Molina + Molina /1978/	1998.2	to 4500.0
CH_3CCl_3	$+ h\nu \rightarrow 3ClO$	$+ CO + CH_3$	Molina + Molina /1978/	1998.2	to 4500.0
			Seery + Britton /1964/	2395.5	to 4500.0
			Hochanadel et al. /1977/	2051.5	to 2920.0
			Cox + Derwent /1976/	2026.0	to 3900.0
			Stockwell + Calvert /1978/	3140.0	to 3900.0
			Cox + Derwent /1976/	2026.0	to 3900.0
			Stockwell + Calvert /1978/	3140.0	to 3900.0
			Molina + Molina /1980/	1846.5	to 3300.0
			Wine /1981/	2797.5	to 3600.0
			Hubrich + Stuhl /1980/	1846.5	to 2548.0

Table 5: Parameters of the quantum yield of photo-dissociation reactions.
For λ_0 a linear approximation of the temperature dependency is
applied: $\lambda_0 = a + b \cdot T$

Reaction	a [nm]	b [nm/K]	$\Delta\lambda$ [nm]	Reference
$O_3 + hv \rightarrow O(^1D) + O_2$	299.6	0.038	2.0	Fairchild + Lee (1978)
$NO_3 + hv \rightarrow NO_2 + O$	597.0		13.0	Magnotta + Johnston (1980)
$NO_3 + hv \rightarrow NO + O_2$	see appendix A.3			Johnston (1983)
$NO_2 + hv \rightarrow NO + O$	403.5		1.0	Okabe (1978)
$SO_2 + hv \rightarrow SO + O$	219.5		1.0	Kelly et al. (1976)
$CO_2 + hv \rightarrow CO + O$	227.4		1.0	Okabe (1978)
$HNO_2 + hv \rightarrow NO_2 + H$	369.0		10.0	Cox + Derwent (1976)
$CH_2O + hv \rightarrow H_2 + CO$	see appendix A.3			Moortgat + Kudzus (1978)
$CH_2O + hv \rightarrow H + CHO$	322.9		4.7	Moortgat et al. (1980)

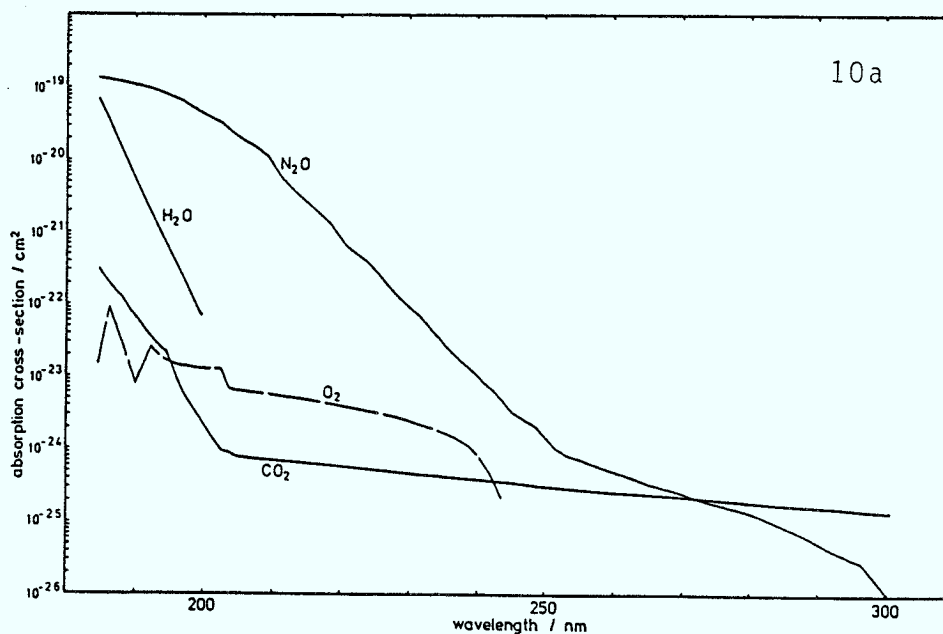
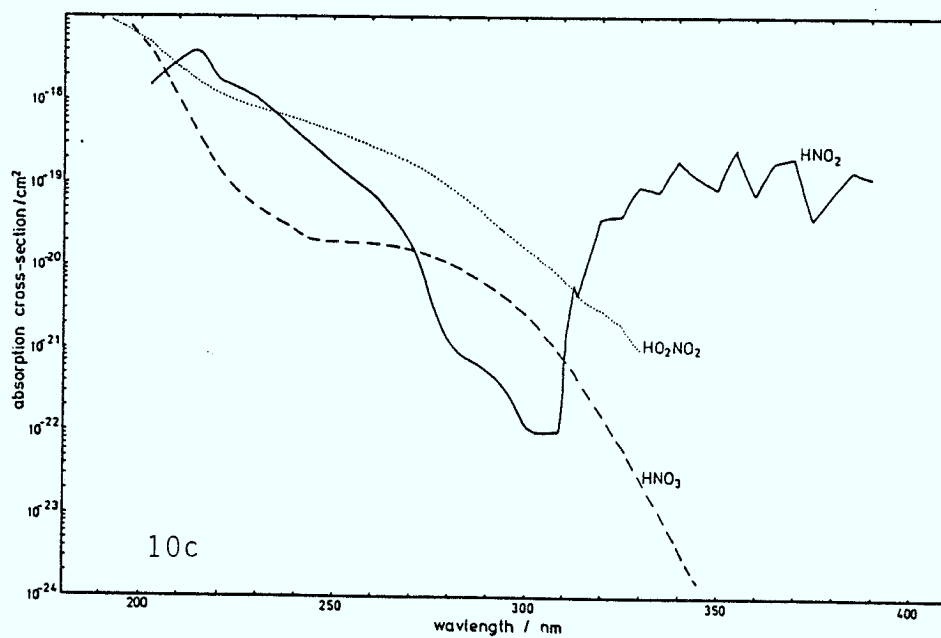
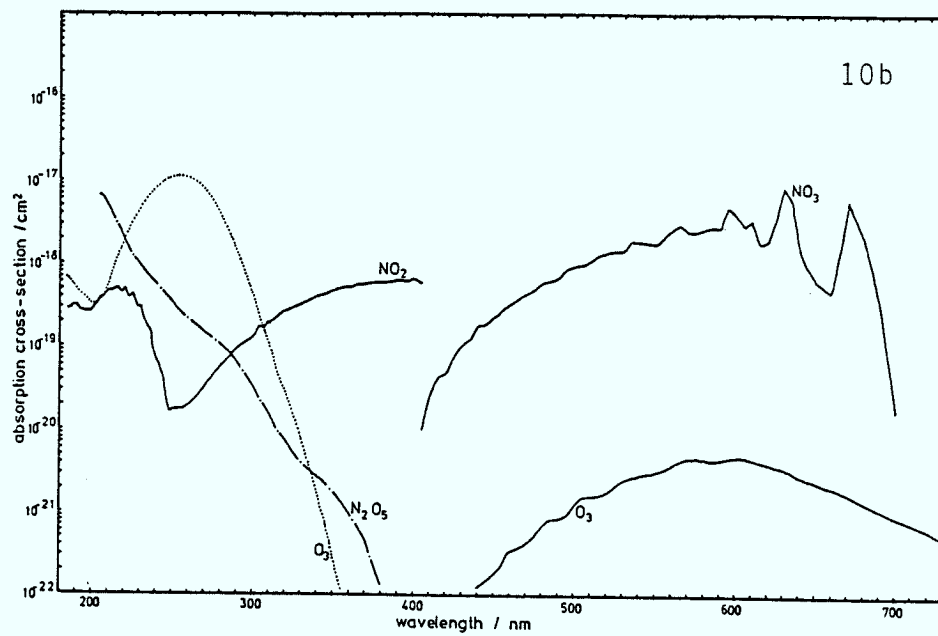
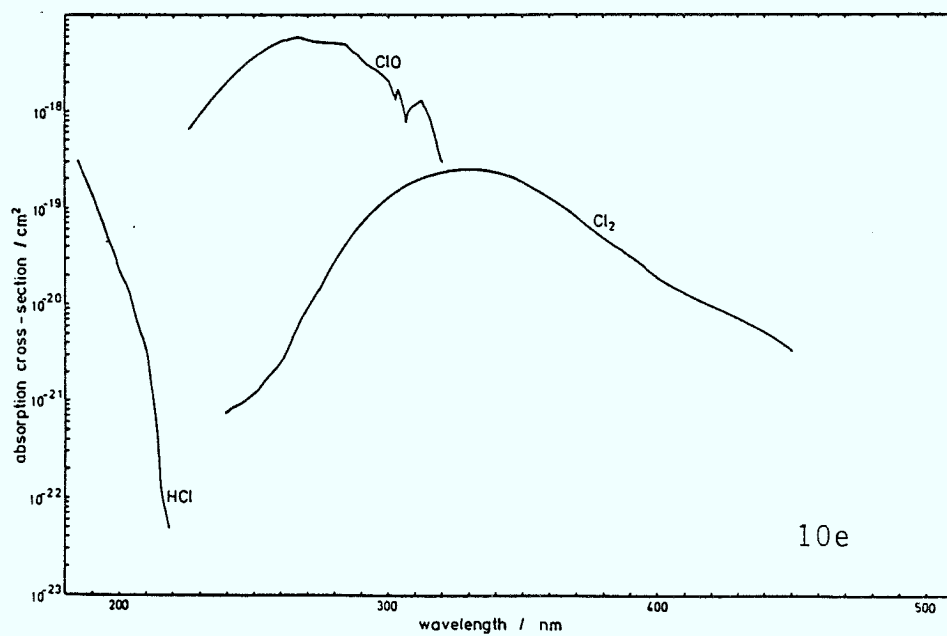
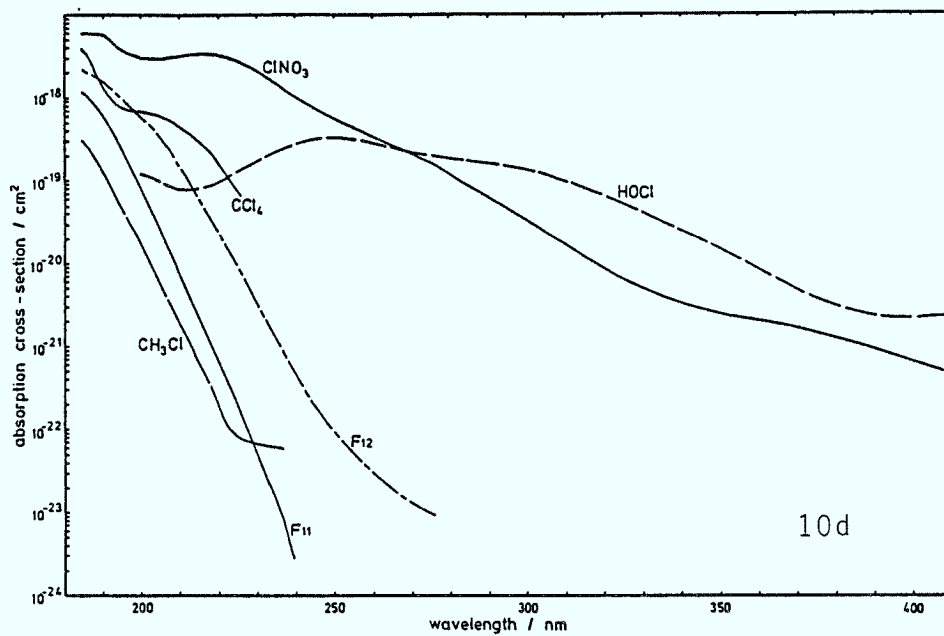
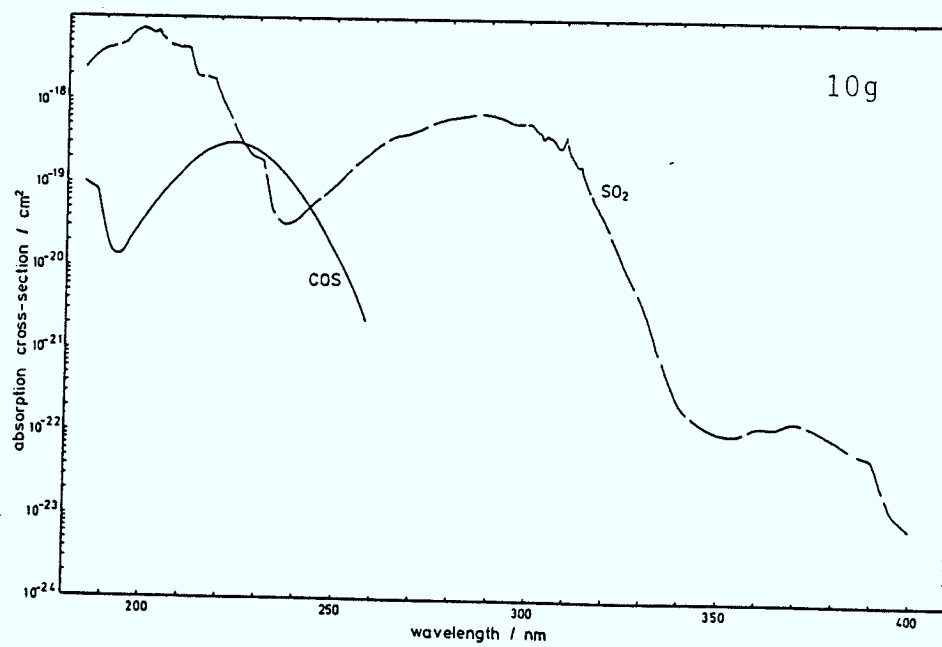
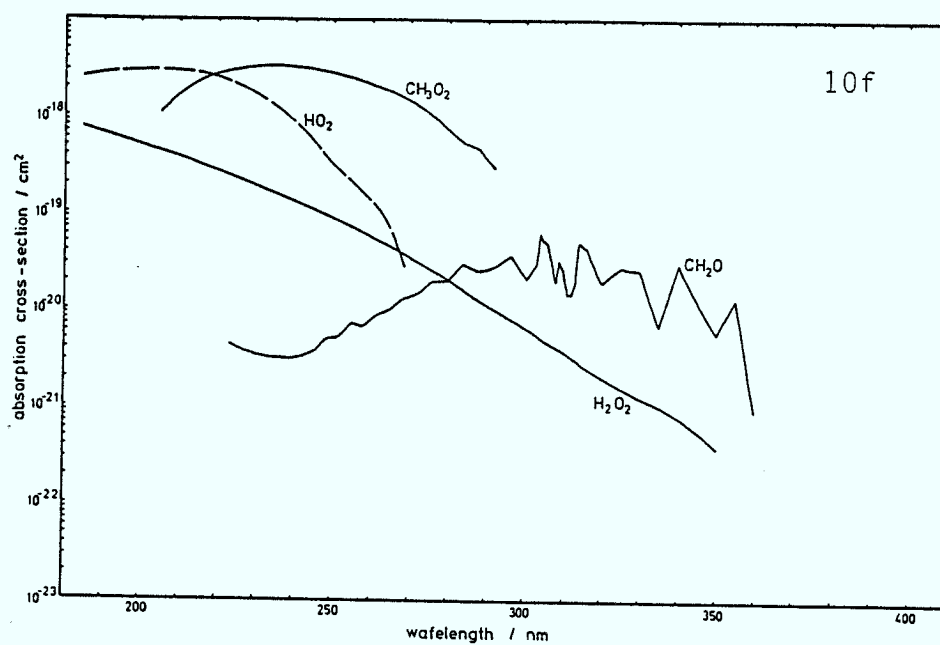


Figure 10: Spectra of the absorption cross-sections used in the
model. The references are listed in table 4.







A.4. Program Listings

As the program flux is straightforward, it is not necessary to include other flux diagrams than those given in fig. 6. Only the subprogram PHOTO is more complicated, so we add its flux diagram to the program listing. The listings of the different subprograms contain extensive comments concerning purpose and input and output parameters, so they are self-explaining and need no further descriptions.

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//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C6,
//      PARM.C='MAP,XREF,OPTIMIZE(2),FIPS(F)',REGION=1536K
//C.SYSIN DD *
```

```
C
C
C          A          000
C          A A        0  0
C          AAAAA      0  0
C          A          A  000
```

```
C *****
C *
C *   MAIN PROGRAM FOR MODEL-CALCULATIONS
C *
C *****
```

```
C PURPOSE          : MAIN PROGRAM, WHICH CALLS THE DIFFERENT
C                   SUBPROGRAMS ACCORDING TO THE CONTROLL-DATA
C INPUT FROM CARDS : ITYP: TYP OF VERSION: =1 STEADY STATE
C                                     =2 LONGTERM VERSION
C                                     =3 DIURNAL VARIATIONS
C                   ITEND,NTAG,NJAHR: NUMBER OF ITERATIONS,DAYS AND
C                                     YEARS TO BE CALCULATED
C                   IDH: ALTITUDINAL STEP
C                   ISUB: NUMBER OF SUBSTANCE TO BE KEPT CONSTANT
C                   IRATE: SWITCH =0: NO OUTPUT OF INDIVIDUAL RATES
C                           =1: OUTPUT OF INDIVIDUAL RATES AFTER
C                               THE N.TH ITERATION
C                   IRAIN: SWITCH =0: NO WET CHEMISTRY AND NO CLOUDS
C                           =1: WET CHEMISTRY AND CLOUD ALBEDO
C                   INTOUT: SWITCH FOR INTERMEDIATE OUTPUT
C                   ICHECK: SWITCH FOR INTERNAL CHECKING OF CL
C                           AND H BALANCE
C                   IMEAN: SWITCH FOR CALCULATION OF AVERAGING FACTORS
C                   IRWCNC: SWITCH FOR OUTPUT OF CONCENTRATION PROFILES
C                           ON DISC
C                   IOUTRL: SWITCH FOR THE FORM OF OUTPUT OF RATES
C                   PHW: PH-VALUE OF CLOUDS
C                   DATE: DATE FOR CALCULATION OF THE SOLAR FLUX
C                   PHI: LATITUDE FOR CALCULATION OF THE SOLAR FLUX
C                   TROPO: ALTITUDE OF THE TROPOPAUSE
C INPUT FROM DISC  : TEMP: TEMPERATURE PROFILE
C                   EDD: EDDYDIFFUSION COEFFICIENT PROFILE
C                   AVK: AVERAGING COEFFICIENTS FOR GASPHASE REACTIONS
C                   DD(11,...): AVERAGING COEFFICIENT FOR
C                               PHOTODISSOCIATION REACTIONS
C OUTPUT ON PRINTER: ALL CONTROLL-PARAMETERS
C                   PLGES,HLIGHT: NOX-PRODUCTION AND ALTITUDE BY
C                               LIGHNING
C                   PSSTG,HSST: NOX-PRODUCTION AND ALTITUDE FROM
C                               SUBSONIC TRANSPORT
C                   AM: AIR DENSITY
C                   TEMP: TEMPERATURE PROFILE
C                   EDD: EDDYDIFFUSION COEFFICIENT PROFILE
C                   AVK,DD(11,...): AVERAGING DATA
C                   H2O,WSSR: PROFILE OF WATER VAPOUR AND LIQUID WATER
C                   UMW: NET CONDENSATION OF WATER
C                   FLUSS: FLUX OF WATER VAPOUR
C OUTPUT VIA COMMON: PLIGHT: NOX-PRODUCTION BY LIGHNING
C                   PSST: NOX-PRODUCTION BY SUBSONIC AIRCRAFTS
C                   PRB: PROBABILITY OF NH3-ABSORPTION IN CLOUDS
```

PHW: PH-VALUE OF CLOUDS
 ALPHA,BETA: SIN*SIN,COS*COS OF PHI AND DECL
 EDD: EDDYDIFFUSION PROFILE
 TEMP: TEMPERATURE PROFILE
 DZ: ALTITUDINAL SPACING
 IRAIN: SWITCH FOR INCLUDING WET CHEMISTRY AND
 CLOUD ALBEDO
 VO2,DVO2: COLUMN DENSITY AND DIFFERENTIAL DENSITY
 OF OXYGEN
 VAM,DVAM: COLUMN DENSITY AND DIFFERENTIAL DENSITY
 OF AIR

SUBROUTINE MAINPR

IMPLICIT REAL*8 (A-H,O-Z)

COMMON-BEREICHE

COMMON /ISWCH/ IP(12)
 COMMON /CONC/ C1(0:99,0:33),C2(0:99,1:30)
 COMMON /TERME/ PC1(0:99,2:33), PC2(0:99,1:30),
 * DC1(0:99,2:33), DC2(0:99,1:30), TT(0:99,2:33)
 COMMON /RAIN/ PHW,PVULK(0:99),PLIGHT(0:99),PSST(0:99),PRB(0:99)
 COMMON /ZENITH/ ALPHA,BETA,TAU(0:99)
 COMMON /RATE/ RR(200,0:99),DD(11,70,0:99),RRN(20,0:99),
 * AVK(200,2),NEP(300,6)
 COMMON /RATEAK/ R(200,0:99),D(70,0:99),RN(20,0:99)
 COMMON /MET/ EDD(0:99),TEMP(0:99),DZ
 COMMON /SL/ VO2(0:99),VO3(0:99),VNO2(0:99),VM(0:99),
 * DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)

DIMENSIONEN

DIMENSION DUMMY(14),TEXT(9),AM(0:99),O2(0:99),O3(0:99)
 INTEGER *2 JOB(8)
 INTEGER *4 MONTH(12)
 INTEGER *4 TAG,MONAT,JAHR,STUNDE,MINUTE,SEKUND
 REAL *4 DATE,PHI,TX(4)

EQUIVALENCE

EQUIVALENCE (AM(0),C1(0,0)),(O2(0),C1(0,1)),(O3(0),C2(0,3))

DATA ZUWEISUNGEN

DATA MONTH/0,31,59,90,120,151,181,212,243,273,304,334/

PKT(Z)=.121*DEXP(.256*Z-.0436*Z*Z)/(DEXP(2.*(Z-8))+1.)
 CALL DATA
 CALL MASKE
 CALL JOBNAM(JOB)
 CALL ZEITN(TAG,MONAT,JAHR,STUNDE,MINUTE,SEKUND)
 WRITE(11) JOB,TAG,MONAT,JAHR,STUNDE,MINUTE,SEKUND

ASSIGNMENTS

PI=3.1415927
 PRB(1)=1.

```

X1=0.
PLGES=0.
PSSTG=0.
PVULG=0.
IENDM=99
DO 89 I=0,IENDM-1
  Z=I
  IF (I.GT.10) GOTO 85
  X=PKT(Z)+PKT(Z+1.)+4.*(PKT(Z+.1)+PKT(Z+.3)+PKT(Z+.5)+PKT(Z+.7)+
1  PKT(Z+.9))+2.*(PKT(Z+.2)+PKT(Z+.4)+PKT(Z+.6)+PKT(Z+.8))
  X1=X1+X/60.
  X=(1.-X1)/(Z+1.5)**2
85 PRB(I+1)=X
  IF (I.LT.11) PLIGHT(I)=6.E3/(SQRT(2.*PI)*2.2)*EXP(-(Z-4.5)**2/
*      (2.*2.2**2))
  IF (I.LT.16) PSST(I)=8.E2/(SQRT(2.*PI)*1.0)*EXP(-(Z-10.)**2/
*      (2.*1.0**2))
  RNN=.075
  AV=.21
  HMAX=1.5
  PRODV=1.5D+03
  X=(RNN/2.)*(Z/HMAX)**2
  PVULK(I)=PRODV*AV*EXP(-X)*(Z/HMAX)**RNN
  PLGES=PLGES+PLIGHT(I)
  PSSTG=PSSTG+PSST(I)
  PVULG=PVULG+PVULK(I)
89 CONTINUE
  DZ=1.E+05
  PLGES=PLGES*DZ
  PSSTG=PSSTG*DZ
  PVULG=PVULG*DZ
  HLIGHT=4.5
  HSST=10.
  ILAUF=1

C
C INPUT OF CONTROLL DATA
C -----
C
WRITE (6,2030)
READ (5,1900) ITYP,ITEND,NTAG,NJAHR,IDH,IEND
READ (5,1900) IP
IRAIN=IP(1)
ISUB=IP(4)
IF (ITYP.EQ.1) WRITE (6,2040) ITEND
IF (ITYP.EQ.2) WRITE (6,2042) NJAHR
IF (ITYP.EQ.3) WRITE (6,2041) NTAG
IF (ISUB.LT.2) WRITE (6,2050)
IF (ISUB.GT.1) WRITE (6,2051) ISUB
WRITE (6,1800) IDH
READ (5,1950) PHW,DOBS
IF (IRAIN.EQ.1) WRITE (6,2000) PHW
IF (IRAIN.EQ.0) WRITE (6,2001)
PHW=10.**(-PHW)
IF (DOBS.NE.0.DO) WRITE (6,2010) DOBS
READ (5,1950) DATE,PHI,TROPO
WRITE (6,2060) DATE,PHI,TROPO
WRITE(11) ITYP,ITEND,NTAG,NJAHR,IDH,IRATE,IRAIN,PHW,DATE,PHI,TROPO
ITAG=(DATE-INT(DATE)+.005)*100.
DECL=-23.44*DCOS((MONTH(ITAG)+INT(DATE)+10.)*2.*PI/365.)
PHIR=PHI*PI/180.
DECLR=DECL*PI/180.
ALPHA=DSIN(PHIR)*DSIN(DECLR)
BETA=DCOS(PHIR)*DCOS(DECLR)

```

```

SUNSET=12.
IF (ALPHA.LT.0.DO) SUNSET=0.
IF (DABS(ALPHA/BETA).LE.1.DO) SUNSET=DARCOS(-ALPHA/BETA)*12./PI
I=SUNSET
Y=(SUNSET-I)*.6
SUNST=I+Y+12.
WRITE (6,1500) SUNST
JOBNR=STUNDE*100+MINUTE
WRITE (6,1600) JOB,JOBNR,TAG,MONAT,JAHR
C
C INPUT OF CONCENTRATION-PROFILES AND METEOROLOGICAL DATA
C -----
CALL RWCONC (1)
CALL SAEUL (DZ,O3,VO3,DVO3)
FACT=2.687D16*DOBS/VO3(0)
IF (DOBS.EQ.0.DO) FACT=1.
DO 91 I=0,IENDM
O3(I)=O3(I)*FACT
C1(I,2)=C2(I,1)+C2(I,2)+C2(I,3)
C1(I,3)=C2(I,4)+C2(I,5)+C2(I,6)+C2(I,7)+C2(I,8)+C2(I,9)+C2(I,10)+
1 C2(I,22)
C1(I,4)=C2(I,9)+C2(I,10)+C2(I,11)+C2(I,12)+C2(I,13)+C2(I,21)
C1(I,5)=C2(I,14)+C2(I,15)
C1(I,6)=C2(I,16)+C2(I,17)
C1(I,7)=C2(I,18)+C2(I,19)+C2(I,20)+C2(I,21)+C2(I,22)
C1(I,8)=C2(I,23)+C2(I,24)+C2(I,25)+C2(I,26)+C2(I,27)
RI=I
C1(I,9)=2.5D2*DEXP(-RI/7.5)
91 CONTINUE
C CALL OUTPT (0.,2,1,99,1)
READ (10,1200) TEXT
WRITE (6,2100) TEXT
READ (10,1300) TEMP
READ (5,1260) NR,(TEXT(I),I=1,8)
WRITE(6,2100) (TEXT(I),I=1,8)
READ (5,1200) TEXT
IF (NR.EQ.0) GOTO 92
READ (5,1300) TEMP
C
C INPUT OF EDDY-COEFFICIENTS
C -----
92 READ (10,1200) TEXT
WRITE (6,2100) TEXT
READ (10,1300) EDD
READ (5,1260) NR,(TEXT(I),I=1,8)
WRITE(6,2100) (TEXT(I),I=1,8)
READ (5,1200) TEXT
IF (NR.EQ.0) GOTO 93
READ (5,1300) EDD
93 CONTINUE
EDD(0)=EDD(1)*AM(1)*EDD(2)*AM(2)/AM(0)/(2.*EDD(2)*AM(2)
* -EDD(1)*AM(1))
EDD(99)=1.E+06
ITRO=TROPO
DO 130 I=4,ITRO+2
EDD(I)=EDD(3)
IF (I.LT.(ITRO-2)) GOTO 130
X=DLOG(EDD(3)/EDD(ITRO+3))/(DEXP(1.5*(I-TROPO))+1.)
EDD(I)=DEXP(X)*EDD(ITRO+3)
130 CONTINUE
DO 135 I=50,IENDM
EDD(I)=EDD(99)*DEXP(DLOG(EDD(50)/EDD(99))/49.*(99.-I))
135 CONTINUE

```

```

CALL SMXRT
C
C INPUT OF BOUNDARY CONDITIONS
C -----
CALL BCOND
WRITE (6,1700) PLGES,HLIGHT,PSSTG,HSST,PVULG,HMAX
C
C OUTPUT OF INPUT-DATA
C -----
IS=2
WRITE(11) IS
WRITE(11) TEMP
WRITE(11) EDD
WRITE(11) C1
WRITE(11) C2
C
C INPUT OF REACTION COEFFICIENT,SOLAR FLUX AND SPECTRAL DATA
C -----
CALL REAKT (AM)
CALL SPEC DT
C
C CALCULATION OF PHOTON FLUX AND PHOTOLYSIS RATES
C -----
CALL SAEUL (DZ,AM,VM,DVM)
CALL SAEUL (DZ,O2,VO2,DVO2)
IF (ITYP.EQ.3) CALL DISMAT
C
C CALCULATION OF WASH-OUT COEFFICIENTS
C -----
CALL WETRM (TROPO)
C
C INPUT OF AVERAGING COEFFICIENTS
C -----
READ (10,1200) TEXT
WRITE (6,2100) TEXT
READ (10,2200) ((AVK(J,1),AVK(J,2)),J=1,200)
READ (10,1260) JE,(TEXT(I),I=1,8)
WRITE (6,2100) (TEXT(I),I=1,8)
DO 209 J=1,JE
READ (10,1260) N
IF (N.NE.J) WRITE (6,1400) N,J
READ (10,1300) (DUMMY(K),K=1,14)
DUMMY(14)=DUMMY(13)
DD(11,J,0)=DUMMY(1)
DO 207 I=1,65
K=(I+4)/5
DD(11,J,I)=DUMMY(K)+(DUMMY(K+1)-DUMMY(K))/5.*(I-5*K+3)
207 CONTINUE
DO 208 I=66,IENDM
DD(11,J,I)=DUMMY(14)
208 CONTINUE
209 CONTINUE
C
IS=5
WRITE(11) IS
WRITE(11) AVK
WRITE(11) ((DD(11,J,I),J=1,70),I=0,IEND)
C
C
C
C BRANCHING
C -----

```

```

C      CALL STEADY (ITEND)
      IF (ITYP.EQ.2) CALL LONGTM (NJAHR)
      IF (ITYP.EQ.3) CALL DIURNL (NTAG, IDH, IEND)

C
C      OUTPUT
C      -----
C
      IF (IP(8).EQ.1) CALL RWCONC (2)
C      IP(8): IRWCNC=1 : OUTPUT ON CARDS
      ILAUF =ILAUF+1
      IF (ILAUF.NE.1) RETURN
99999 RETURN
C
C      FORMATS
C      -----
C
1200 FORMAT (9A8)
1260 FORMAT (I3,8A8)
1300 FORMAT (7(1P,E10.3))
1400 FORMAT ('0 ERROR PHOTOLYSIS AVERAGE : N=',I5,' NE J=',I5/)
1500 FORMAT (' SUNSET AT',F6.2,'HR'/)
1600 FORMAT ('0 JOB NR.: ',8A2,I8,10X,'FROM ',I3,I3,I3)
1700 FORMAT('0 NOX-PRODUCTION BY LIGHTNING:',1P,E9.2,'CM-2 S-1 AROUND'
* ,OP,F5.1,'KM'/17X,'BY AIRCRAFTS:',1P,E9.2,'CM-2 S-1 AROUND',OP
* ,F5.1,'KM'/' SO2-PRODUCTION BY VULCANOES:',1P,E9.2,'CM-2 S-1
*AROUND',OP,F5.1,'KM')
1800 FORMAT ('0 ALTITUDINAL STEP =',I3,'KM')
1900 FORMAT (6(7X,I5))
1950 FORMAT (6(7X,F5.2))
2000 FORMAT ('0 PH-VALUE OF CLOUDS =',F4.1,10X,'RAIN ACTIVATED')
2001 FORMAT ('0 WITHOUT RAIN')
2010 FORMAT ('0 OZONE-COLUMN-DENSITY SET TO',F5.0,'DOBSON')
2020 FORMAT (I5,1P,10E12.2)
2030 FORMAT ('1 PARAMETERS '/16('=')/)
2040 FORMAT ('0 CALCULATION OF STEADY-STATE VERSION FOR',I4,
* ' ITERATIONS'/)
2041 FORMAT ('0 CALCULATION OF DIURNAL VARIATION FOR',I3,' DAYS'/)
2042 FORMAT ('0 CALCULATION OF THE LONGTERM VERSION FOR',I4,' YEARS'/)
2050 FORMAT ('0 ALL COMPOUNDS ARE CALCULATED'/)
2051 FORMAT ('0 COMPOUND NR.',I3,' IS KEPT CONSTANT'/)
2060 FORMAT ('0 DATUM =',F6.2/' BREITENGRAD =',F6.2/
* ' TROPOPAUSE =',F6.2)
2100 FORMAT ('0',10A8)
2200 FORMAT (3(4X,2E10.2))
      END
/*

```

```
//ICH301A1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C6,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          A          1
C        A A      1  1
C       AAAAA      1
C        A      A      1
C
```

```
C *****
C *
C *   UNTERGROGRAMM: DATA INITIALIZATION   *
C *
C *****
```

```
C PURPOSE   : INITIALIZING OF THE COMMON-REGIONS
```

```
C
C   SUBROUTINE DATA
```

```
C   =====
```

```
C   IMPLICIT REAL*8 (A-H,O-Z)
```

```
C   COMMON
```

```
C   -----
```

```
C   COMMON /RAIN /   PHW,PV(100),PL(100),PS(100),PR(100)
C   COMMON /ZENITH/  ALPHA,BETA,TAU(100)
C   COMMON /YIELD/   XLAM0(140),DLAM(140),SLYM(70),TFAK(7000)
C   COMMON /RATEAK/  RTAK(29000)
C   COMMON /RATE/    RT(99400),NEP(1800)
C   COMMON /TERME/   TRM(15600)
C   COMMON /CONC/    C(6400),ISUB
C   COMMON /ISO/     Y(85800)
```

```
C   INITIALIZING
```

```
C   -----
```

```
C
C   DO 19 J=1,70
C       XLAM0(J)   =0.
C       XLAM0(J+70)=0.
C       DLAM (J)   =0.
C       DLAM (J+70)=0.
C       SLYM (J)=0.
C   DO 19 I=1,100
C       TFAK ((J-1)*100+I)=1.
19  CONTINUE
C   DO 29 I=1,100
C       TAU(I)=1.
C       PV(I)=0.
C       PL(I)=0.
C       PS(I)=0.
C       PR(I)=0.
C   DO 21 J=1,18
C       RTAK(I+(J-1)*100)=0.
C       RT (I+(J-1)*100)=0.
C       NEP(I+(J-1)*100)=0
C       TRM(I+(J-1)*100)=0.
C       C (I+(J-1)*100)=0.
C       Y (I+(J-1)*100)=0.
21  CONTINUE
```

```
DO 22 J=19,64
  RTAK(I+(J-1)*100)=0.
  RT (I+(J-1)*100)=0.
  TRM(I+(J-1)*100)=0.
  C  (I+(J-1)*100)=0.
  Y  (I+(J-1)*100)=0.
22  CONTINUE
DO 23 J=65,156
  RTAK(I+(J-1)*100)=0.
  RT (I+(J-1)*100)=0.
  TRM(I+(J-1)*100)=0.
  Y  (I+(J-1)*100)=0.
23  CONTINUE
DO 24 J=157,290
  RTAK(I+(J-1)*100)=0.
  RT (I+(J-1)*100)=0.
  Y  (I+(J-1)*100)=0.
24  CONTINUE
DO 25 J=291,858
  RT (I+(J-1)*100)=0.
  Y  (I+(J-1)*100)=0.
25  CONTINUE
DO 26 J=859,994
  RT (I+(J-1)*100)=0.
26  CONTINUE
29  CONTINUE
RETURN
END
/EOF
/EOD
```

```
//ICH301B1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,15)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B1,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C          BBB          1
C          B__B      1 1
C          B__B          1
C          BBB          1
C
C *****
C *                                     *
C *  UNTERGROGRAMM: READ/WRITE CONCENTRATIONS  *
C *                                     *
C *****
C
C PURPOSE          : INPUT OF CONCENTRATIONS FROM DISK AND CARDS
C                   AND OUTPUT ON CARDS
C INPUT VIA CALL   : N : SWITCH    =1 INPUT
C                   =2 OUTPUT ON CARDS
C INPUT FROM DISC  : TEXT1 : HEADING
C                   AND CARDS NR   : INDEX OF COMPONENT
C                   TEXT2 : NAME OF COMPONENT
C                   C      : CONCENTRATION PROFILE
C OUTPUT VIA COMMON: C      : CONCENTRATION PROFILE
C OUTPUT ON CARDS  : J      : INDEX OF COMPONENT
C                   C      : CONCENTRATION PROFILE
C OUTPUT ON PRINTER: TEXT1 : HEADING
C                   TEXT2 : NAME OF COMPONENT TO BE READ IN FROM CARDS
C
C      SUBROUTINE RWCONC (N)
C      =====
C
C      COMMON - BEREICHE
C      -----
C      COMMON /CONC/ C
C
C      DIMENSIONS
C      -----
C      REAL*8 TEXT(8),C(0:99,0:63)
C
C      FORMATS
C      -----
C      1100 FORMAT (I3,8A8)
C      1200 FORMAT (8A8)
C      1250 FORMAT ('0',9A8)
C      1300 FORMAT (1P,7E10.3)
C      2100 FORMAT (I4,8A8)
C      2300 FORMAT (1X,1P,7E10.3)
C
C      READING
C      -----
C      IF (N.NE.1) GOTO 20
C      READ (10,1100) NRX,TEXT
C      WRITE (6,1250) TEXT
C      DO 9 J=1,NRX
C          READ (10,1100) NR,TEXT
C          READ (10,1300) (C(I,NR),I=0,99)
C      9  CONTINUE
C      10 CONTINUE
C          READ (5,1100) NR,TEXT
```

```
        WRITE (6,1250)  TEXT
        READ (5,1200) TEXT
        READ (5,1200) TEXT
        IF (NR.EQ.0) RETURN
        READ (5,1300) (C(I,NR),I=0,99)
    GOTO 10
C
C    PUNCHING
C    -----
20 CONTINUE
    IF (N.NE.2) RETURN
    DO 29 J=11,60
        WRITE (9,2100) J
        WRITE (9,2300) (C(I,J),I=0,99)
29 CONTINUE
C
30 CONTINUE
    RETURN
    END
/*
```

//ICH301B2 JOB (324,035431),ROETH,CLASS=C,TIME=(00,15)

/*PASSWORD MODEL

/*ROUTE PRINT CMS.ICH301

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B2,

// PARM.C='MAP,XREF,OPTIMIZE(2),FIPS(F)'

//C.SYSIN DD *

C

C

C

C

C

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C

C

C

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BBB 22
B B 2 2
B B 2
BBB 2222

* *

* UNTERGROGRAMM: BOUNDARY CONDITIONS *

* *

PURPOSE : INPUT OF BOUNDARY CONDITIONS FROM DISC (STANDARD)
AND CARDS

INPUT VIA COMMON : AMO,AM99: AIR DENSITY AT 0 AND 99 KM ALTITUDE

EDD : EDDY DIFFUSION COEFFICIENT

INPUT FROM DISK : NR : NUMBER OF COMPONENTS FOR WHICH BOUNDARY
CONDITIONS ARE TO BE READ IN

TEXT1 : HEADING

I : INDEX OF THE COMPONENT

PO : MIXING RATIO AT THE LOWER BOUNDARY

VO : DEPOSITION VELOCITY AT 0 KM ALTITUDE

PROD : PRODUCTION RATE AT THE LOWER BOUNDARY

P1 : MIXING RATIO AT 99 KM ALTITUDE

TEXT2 : NAME OF THE COMPONENT

OUTPUT VIA COMMON: X(0,I) : MIXING RATIOS AT 0 KM

X(99,I) : MIXING RATIOS AT 99 KM

XMR : MIXING RATIOS AT GROUND LEVEL

PRD : PRODUCTION FLUXES AT GROUND LEVEL

VDP : DEPOSITION VELOCITY

OUTPUT ON PRINTER: ALL INFORMATION READ IN AND CALCULATED

REMARKS : NR=0 ENDS THE INPUT FROM CARDS

(2 ADDITIONAL CARDS AS DUMMY HEADING NECESSARY)

SUBROUTINE BCOND

IMPLICIT REAL*8 (A-H,O-Z)

COMMON-BEREICHE

COMMON /CONC / C(0:99,0:63)

COMMON /MET / EDD(0:99),TEMP(0:99),DZ

COMMON /BNDC / XMR(33),PRD(33),VDP(33),X99(33)

DIMENSIONS

REAL*8 TEXT(9)

IS=0

AMO= C(0,0)

AM99=C(99,0)

READ (10,1100) NR,TEXT

WRITE (6,2000) TEXT

2 CONTINUE

DO 9 J=1,NR

IF (IS.EQ.0) READ (10,1000) I,PO,VO,PROD,P1,TEXT(1)

```
      IF (IS.EQ.1) READ (5,1000) I,P0,V0,PROD,P1,TEXT(1)
      IF (P0.NE.0) C( 0,I)=P0*AM0
      C(99,I)=P1*AM99
      X99(I)=P1
      WRITE (6,2100) I,P0,V0,PROD,P1,TEXT(1)
      XMR(I)=P0
      PRD(I)=PROD
      VDP(I)=V0
9     CONTINUE
      IS=1
      READ (5,1100) NR,TEXT
      WRITE (6,1300) TEXT
      READ (5,1200) TEXT
      READ (5,1200) TEXT
      IF (NR.NE.0) GOTO 2
      WRITE (6,2200)
      RETURN
1000 FORMAT (I3,1P,E9.2,0P,F5.2,1P,2E9.2,A8)
1100 FORMAT (I3,9A8)
1200 FORMAT (9A8)
1300 FORMAT ('0',9A8)
2000 FORMAT ('1',9A8//' ! NR ! X(0) ! V(0) ! PROD !
*      , ' X(100) !'/1X,65('='))
2100 FORMAT (' ! ',I4,4(' ! ',1P,E10.2),' ! ',A8,' ! ')
2200 FORMAT (/ '0 X = MIXING RATIO'/' PROD= PRODUCT.FLUX'/
*      ' V(0)= DEPOSIT.VELOCITY')
      END
/*
```

```
//ICH301B3 JOB (324,035431),ROETH,CLASS=C,TIME=(00,15)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B3,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C                                     BBB      333
C                                     B  B      3
C                                     B  B      3
C                                     BBB      333
C
C *****
C *                                     *
C *   UNTERPROGRAMM SMXRT : SUM MIXING RATIOS   *
C *                                     *
C *****
C
C PURPOSE          : SETTING MIXING RATIOS OF ALL GROUP MEMBERS AT
C                   GROUND LEVEL AND AT 98 KM EQUAL TO THOSE AT 1 KM
C                   AND 97 KM, RESP., WITHOUT CHANGING THE
C                   APPROPRIATE GROUP CONCENTRATION
C INPUT AND OUTPUT VIA COMMON : X: CONCENTRATION PROFILES
C
C   SUBROUTINE SMXRT
C   =====
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C   COMMON-BEREICHE
C   -----
C   COMMON /CONC/ C1(0:99,0:33),C2(0:99,1:30)
C
C   IEND=99
C
C   DO 9 J=1,30
C       C2(0,J)= C2(1,J)/C1(1,0)*C1(0,0)
C       C2(IEND,J)=C2(IEND-1,J)/C1(IEND-1,0)*C1(IEND,0)
9 CONTINUE
DO 19 I=0,IEND,IEND
Y=C1(I,2)/(C2(I,1)+C2(I,2)+C2(I,3))
C2(I,1)=C2(I,1)*Y
C2(I,2)=C2(I,2)*Y
C2(I,3)=C2(I,3)*Y
Y=C1(I,3)/(C2(I,4)+C2(I,5)+C2(I,6)+C2(I,7)+C2(I,8)+C2(I,9)+
*      C2(I,10)+C2(I,22))
C2(I,4)=C2(I,4)*Y
C2(I,5)=C2(I,5)*Y
C2(I,6)=C2(I,6)*Y
C2(I,7)=C2(I,7)*Y
C2(I,8)=C2(I,8)*Y
C2(I,9)=C2(I,9)*Y
C2(I,10)=C2(I,10)*Y
C2(I,22)=C2(I,22)*Y
Y=C1(I,4)/(C2(I,9)+C2(I,10)+C2(I,11)+C2(I,12)+C2(I,13)+
*      C2(I,21))
C2(I,9)=C2(I,9)*Y
C2(I,10)=C2(I,10)*Y
C2(I,11)=C2(I,11)*Y
C2(I,12)=C2(I,12)*Y
C2(I,13)=C2(I,13)*Y
C2(I,21)=C2(I,21)*Y
Y=C1(I,5)/(C2(I,14)+C2(I,15))
```

```
C2(I,14)=C2(I,14)*Y
C2(I,15)=C2(I,15)*Y
Y=C1(I,6)/(C2(I,16)+C2(I,17))
C2(I,16)=C2(I,16)*Y
C2(I,17)=C2(I,17)*Y
Y=C1(I,7)/(C2(I,18)+C2(I,19)+C2(I,20)+C2(I,21)+C2(I,22))
C2(I,18)=C2(I,18)*Y
C2(I,19)=C2(I,19)*Y
C2(I,20)=C2(I,20)*Y
C2(I,21)=C2(I,21)*Y
C2(I,22)=C2(I,22)*Y
Y=C1(I,8)/(C2(I,23)+C2(I,24)+C2(I,25)+C2(I,26)+C2(I,27))
C2(I,23)=C2(I,23)*Y
C2(I,24)=C2(I,24)*Y
C2(I,25)=C2(I,25)*Y
C2(I,26)=C2(I,26)*Y
C2(I,27)=C2(I,27)*Y
```

```
19 CONTINUE
```

```
RETURN
```

```
END
```

```
/*
```

//ICH301B4 JOB (324,035431),ROETH,CLASS=C,TIME=(00,59)

/*PASSWORD MODEL

/*ROUTE PRINT MVS

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B4,

// PARM.C='MAP,XREF,OPTIMIZE(2)'

//C.SYSIN DD *

C

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```

BBB      4      4
B  B     4      4
B  B     44444
BBB      4

```

```

*****
*
*   UNTERPROGRAMM: INPUT OF THE COMPONENTS
*                   OF THE REACTION CONSTANTS
*
*****

```

```

C PURPOSE          : INPUT OF THE PARAMETERS OF THE REACTION
C                   COEFFICIENTS FROM DISC AND CARDS AND
C                   CALCULATION OF THE ALTITUDINAL DEPENDENCE
C                   OF THE RATE COEFFICIENTS
C INPUT VIA CALL    : AM: AIR DENSITY
C INPUT VIA COMMON  : TEMP: TEMPERATURE PROFILE
C INPUT FROM DISC   : NR: NUMBER OF REACTIONS TO BE READ IN
C                   TEXT1: HEADING
C                   J1: INDEX OF THE REACTION
C                   BIMOLECULAR REACTIONS :
C                   G1: PREEXPONENTIAL FACTOR
C                   E1: ACTIVATION TEMPERATURE
C                   NX: SYMBOL OF THE REACTION PARTNERS AND PRODUCTS
C                   TEXT2: REACTION EQUATION
C                   TRIMOLECULAR REACTIONS :
C                   G1,G2: RATE COEFFICIENT AT 300K AND 1 ATM
C                   E1,E2: EXPONENT OF THE TEMPERATURE DEPENDENCE
C                   WET CHEMISTRY REACTIONS :
C                   G: RATE COEFFICIENT OR EQUILIBRIUM CONSTANT
C                   E: ACTIVATION TEMPERATURE OF G
C OUTPUT ON PRINTER: ALL DATA READ IN AND THE RATE COEFFICIENTS AT
C                   GROUND LEVEL
C OUTPUT VIA COMMON: R,RN: PROFILES OF THE RATE COEFFICIENTS FOR
C                   GASPHASE AND WET REMOVAL REACTIONS

```

SUBROUTINE REAKT (AM)

=====

COMMON

```

COMMON /MET/      EDD(0:99),TEMP(0:99),DZ
COMMON /RATE/     R(200,0:99),D(11,70,0:99),RN(20,0:99),
1                AVK(200,2),NEP(300,6)

```

DIMENSION

```

REAL*8 AM(0:99),TEXT( 4),R,D,RN,AVK,EDD,TEMP,DZ
INTEGER*4 NX(6)

```

GAS - PHASE

BIMOLEKULARE REAKTIONEN

IS=0

IEND=99

```

      READ (10,1300) NR,TEXT
      WRITE (6,2000) TEXT
12  DO 10 J=1,NR
      IF (IS.EQ.0) READ (10,1000) J1,G1,E1,(NX(I),I=1,6),TEXT
      IF (IS.EQ.1) READ (5,1000) J1,G1,E1,(NX(I),I=1,6),TEXT
          DO 20 I=0,IEND
              R(J1,I)=G1*DEXP(E1/TEMP(I))
20      CONTINUE
          DO 22 I=1,6
22      NEP(J1,I)=NX(I)
          WRITE (6,2100) J1,G1,E1,R(J1,0),(NEP(J1,I),I=1,6),TEXT
10  CONTINUE
      IS=1
      READ (5,1300) NR,TEXT
      WRITE (6,1400) TEXT
      READ (5,1500) TEXT
      READ (5,1500) TEXT
      IF (NR.NE.0) GOTO 12

```

C

C

```

      TERMOLEKULARE REAKTIONEN
      IS=0
      READ (10,1300) NR,TEXT
      WRITE (6,2400) TEXT
32  DO 38 J=1,NR
      IF (IS.EQ.0) READ (10,1200) J1,G1,E1,G2,E2,(NX(I),I=1,6),TEXT
      IF (IS.EQ.1) READ (5,1200) J1,G1,E1,G2,E2,(NX(I),I=1,6),TEXT
          DO 35 I=0,IEND
              X=G1*(300./TEMP(I))**E1*AM(I)
              R(J1,I)=X
              IF (G2.EQ.0.) GOTO 35
              Y=X/(G2*(300./TEMP(I))**E2)
              R(J1,I)=X/(1.+Y)*.6**(1./(1.+(ALOG10(Y))**2))
35  CONTINUE
          DO 36 I=1,6
36  NEP(J1,I)=NX(I)
          WRITE (6,2500) J1,G1,E1,G2,E2,R(J1,0),(NEP(J1,I),I=1,6),TEXT
38  CONTINUE
      IS=1
      READ (5,1300) NR,TEXT
      WRITE (6,1400) TEXT
      READ (5,1500) TEXT
      READ (5,1500) TEXT
      IF (NR.NE.0) GOTO 32

```

C

C

```

      NASS - CHEMIE
      IS=0
      READ (10,1300) NR,TEXT
      WRITE (6,2200) TEXT
52  DO 50 J=1,NR
          IF (IS.EQ.0) READ (10,1100) J1,G,E,TEXT
          IF (IS.EQ.1) READ (5,1100) J1,G,E,TEXT
              DO 40 I=0,IEND
                  RN(J1,I)=G*DEXP(E/TEMP(I))
40      CONTINUE
          WRITE (6,2300) J1,G,E,RN(J1,0),TEXT
50  CONTINUE
      IS=1
      READ (5,1300) NR,TEXT
      WRITE (6,1400) TEXT
      READ (5,1500) TEXT
      READ (5,1500) TEXT
      IF (NR.NE.0) GOTO 52

```

C

```

DO 69 I=3,IEND
R(190,I)=0.
69 CONTINUE
C
    RETURN
C
2000 FORMAT ('1',4A8// ' K=A*EXP(T0/T)'//
*          ' NR',5X,'A',8X,'T0',4X,'REACT.CONST.',
*          5X,'SYMBOL',15X,'REACTION'/85('='))
1000 FORMAT (I3,E10.2,F6.0,12X,2(I2,1X),A1,3(1X,I2),4A8)
1300 FORMAT (I3,4A8)
1400 FORMAT ('0',4A8)
1500 FORMAT (4A8)
2100 FORMAT (' ',I3,1P,E10.2,0P,F7.0,2X,1P,E10.2,
*          4X,2I3,A2,3I3,8X,4A8)
2200 FORMAT ('1',4A8// ' K=A*EXP(T0/T)'// ' NR',5X,'A',8X,'T0',10X,
*          'CONST.',12X,'REACTION'/85('='))
1100 FORMAT (I3,E10.2,F8.0,26X,4A8)
2300 FORMAT (' ',I3,1P,E10.2,0P,F10.0,3X,1P,E10.2,10X,4A8)
2400 FORMAT ('1',4A8// ' K=K0*(300/T)**N*AM/(1+Y)*.6**(1/(LG(Y))**2
*)' WHITH Y=(K0*(300/T)**N*AM)/(KU*(300/T)**M)'//
*          ' NR',5X,'K0',7X,'N',6X,'KU',7X,'M',5X,'REACT.CONST.',
*          5X,'SYMBOL',10X,'REACTION'/95('='))
1200 FORMAT (I3,2(E10.2,F4.1),2(I2,1X),A1,3(1X,I2),4A8)
2500 FORMAT (' ',I3,2(1P,E10.2,0P,F6.1),3X,1P,E10.2,
*          4X,2I3,A2,3I3,3X,4A8)
END
/*

```

```
// ICH301B5 JOB (324,035431),ROETH,CLASS=C,TIME=(00,19)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B5,
// PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
```

```
C
C
C          BBB      5555
C          B  B      5
C          B  B      5  5
C          BBB      555
```

```
C *****
C *
C *   UNTERPROGRAMM: INPUT OF WAVELENGTHS,
C *                   EXTRATERRISTIC PHOTONFLUXES,
C *                   ABSORPTION-CROSSSECTIONS + QUANTUM YIELDS
C *                   SOLAR SPECTRUM FROM 121.6 NM TO 730 NM
C *
C *****
```

```
C PURPOSE          : INPUT OF THE WAVELENGTH-DEPENDENT DATA: WAVELENGTH,
C                   PHOTONFLUX AND ABSORPTION CROSS-SECTIONS
C INPUT FROM DISC : DEXT: HEADINGS
C                   AND CARDS  WAVE: WAVELENGTH
C                   DELTA: SPACING OF THE SPECTRAL DATA
C                   FLUX: PHOTON FLUX AT 100 KM
C                   IANF,IEND: INDEX OF FIRST AND LAST CROSS-SECTION
C                   ABSS: CROSS-SECTIONS FOR THE ABSORPTION OF THE
C                   PHOTON FLUX (ABSS(4) IS THE REFRACTION NUMBER
C                   OF THE AIR FROM WHICH ABSS(5), THE RAYLEIGH
C                   CROSS-SECTION IS CALCULATED)
C                   RED: COEFFICIENTS FOR THE SCHUMANN-RUNGE BANDS
C                   NR: INDEX OF THE PHOTODISSOCIATION REACTION
C                   SUBST: NAME OF THE COMPONENT TO BE DISSOCIATED
C                   NEPP: SYMBOLS OF THE REACTION PARTNERS AND PRODUCTS
C                   TEXT: REACTION EQUATION
C                   SLY: PHOTODISSOCIATION FREQUENCY OF THE LYMAN LINE
C                   RLAO,RLAIAND DLO,DL1: COEFFICIENTS FOR TEMPERATURE
C                   OR PRESSURE DEPENDENCE OF THE QUANTUM YIELD
C                   STF: COEFFIENTS OF THE TEMPERATURE DEPENDENCE OF
C                   THE ABSORPTION CROSS-SECTIONS
C                   S: CROSS-SECTIONS FOR THE CALCULATION OF THE
C                   PHOTODISSOCIATION FREQUENCIES
C OUTPUT VIA COMMON AND ON PRINTER: ALL SPECTRAL DATA READ IN
```

SUBROUTINE SPECDDT

DIMENSION

COMMON

```
COMMON / RATE / R(200,0:99),D(11,70,0:99),RN(20,0:99),
*          AVK(200,2),NEP(300,6)
COMMON /SPECT / WAVE(130),FLUX(130),S(70,130),ABSS(7,130),
*          RED(8,9),STF(8,70),SUBSTZ(70)
COMMON /YIELD / LAMO(2,70),DLAM(2,70),SLYM(70),TFAK(0:99,70)
```

```
INTEGER*4 NEPP(6)
REAL *8 DEXT(7),WAVE,DELTA(130),FLUX,STF,ABSS,RED,S,LAMO,DLAM,
```

```
1      SLYM,TEXT(4),TEXT1(3),SUBST,SUBSTZ,SLY,LAMCM,
2      R,D,RN,AVK,TFAK
C
      PI=3.1415927
      WRITE (6,2000)
      READ (10,1000) DEXT
      READ (10,1100) WAVE
      WRITE (6,2100) DEXT
      READ (10,1000) DEXT
      READ (10,1100) DELTA
      WRITE (6,2100) DEXT
      READ (10,1000) DEXT
      READ (10,1200) FLUX
      WRITE (6,2100) DEXT
C
C      INPUT OF ABSORPTION-SPECTRA
C      -----
C
      READ (10,1000) DEXT
      WRITE (6,2200) DEXT
      DO 10 I=1,4
        READ (10,1300) IANF,IEND,DEXT
        READ (10,1200) (ABSS(I,J),J=IANF,IEND)
        WRITE (6,2100) DEXT
10 CONTINUE
      AMO=2.547E+19
      DO 19 L=1,130
        ABSS(1,L)=ABSS(1,L)*0.6
        LAMCM=WAVE(L)*1.E-08
        ABSS(5,L)=8.*PI**3*(((ABSS(4,L)+1.)**2-1.)**2/
*          (3.*LAMCM**4*AMO**2))*((6.+3.*.035)/(6.-7.*.035))
19 CONTINUE
C
      IS=31
      WRITE(11) IS
      WRITE(11) WAVE
      WRITE(11) ABSS
      WRITE(11) FLUX
C
      READ (10,1000) DEXT
      WRITE (6,2200) DEXT
      DO 20 K=1,9
        READ (10,1400) (RED(J,K),J=1,8)
20 CONTINUE
C
C      INPUT OF PHOTOLYSIS-SPECTRA
C      -----
C
      READ (10,1000) DEXT
      WRITE (6,2300)
      WRITE (6,2100) DEXT
      WRITE (6,2400)
30 CONTINUE
      READ (10,1500) NR,SUBST,NEPP,TEXT
      IF (NR.EQ.0) GOTO 50
      READ (10,1600) NR,SLY,RLA0,RLA1,DLO,DL1
      READ (10,2600) (STF(I,NR),I=1,4)
      SUBSTZ(NR)=SUBST
      DO 35 I=1,6
35      NEP(200+NR,I)=NEPP(I)
      SLYM(NR)=SLY
      LAM0(1,NR)=RLA0
      LAM0(2,NR)=RLA1
```

```
      DLAM(1,NR)=DL0
      DLAM(2,NR)=DL1
      IX=0
40  READ (10,1800) IA,IE,TEXT1
      IF(IX.EQ.0)WRITE(6,1700)NR,SUBST,NEPP,TEXT,TEXT1,WAVE(IA),WAVE(IE)
      IF (IA.EQ.0) GOTO 30
      IF (IX.EQ.1) WRITE (6,1900) TEXT1,WAVE(IA),WAVE(IE)
      READ (10,1200) (S(NR,I),I=IA,IE)
      IX=1
      GOTO 40
C
50  CONTINUE
      DO 51 J=1,26
51  S(1,J)=S(1,J)*0.6
      IS=32
      WRITE(11) IS
      WRITE(11) S
      WRITE(11) LAMO
      WRITE(11) DLAM
      WRITE(11) STF
C
      RETURN
1000 FORMAT (7A8)
1100 FORMAT (8F8.2)
1200 FORMAT (7E10.3)
1300 FORMAT (2I4,7A8)
1400 FORMAT (6E12.5)
1500 FORMAT (I3,A8,20X,I2,2(1X,A2),2(I2,1X),I2,4A8)
1600 FORMAT (I5,E10.2,2(F10.2,E10.2))
1700 FORMAT (I5,3X,A8,1X,I3,1X,2A2,3I3,3X,7A8,
*          'FROM',F8.1,' TO',F8.1)
1800 FORMAT (2I5,4A8)
1900 FORMAT (69X,3A8,'FROM',F8.1,' TO',F8.1)
2000 FORMAT ('1 HEADINGS OF SPECTRAL DATA READ IN'//)
2100 FORMAT (' ',7A8)
2200 FORMAT ('0',7A8)
2300 FORMAT ('1'/)
2400 FORMAT ('ONR  SUBSTANCE',8X,'SYMBOL',9X,'REACTION',24X,'SPECTRUM'
*          ,16X,'WAVELENGTH REGION'/116('=')/)
2600 FORMAT (8E9.2)
      END
/*
```

```
//ICH301B6 JOB (324,035431),ROETH,CLASS=C,TIME=(00,15)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301B6,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          BBB      666
C          B__B     6
C          B  B     6  6
C          BBB      666
```

```
C
C *****
C *
C *      UNTERPROGRAMM: LIQUID AND GASEOUS WATER      *
C *                      AND NET CONDENSATION          *
C *
C *****
```

```
C PURPOSE          : CALCULATION OF THE GASEOUS WATER CONTENT,OF THE
C                   WET REMOVAL RATE OF WATER AND OF THE LIQUID WATER
C                   CONTENT FROM GROUND LEVEL TO 20 KM ALTITUDE
C INPUT VIA CALL    : TROPO: ALTITUDE OF THE TROPOPAUSE
C INPUT VIA COMMON  : C: CONCENTRATION OF THE AIR
C                   EDD: EDDY-DIFFUSION COEFFICIENT
C                   TEMP: TEMPERATURE PROFILE
C                   DZ: ALTITUDINAL SPACING
C                   PHW: PH-VALUE OF THE CLOUDS
C                   RNN: WET CHEMISTRY DATA
C                   RAINFK: SWITCH  =0: NO RAIN
C                           =1: WET CHEMISTRY ACTIVATED
C INPUT VIA DATA   : FEUCHT: RELATIVE HUMIDITY
C OUTPUT ON PRINTER: RAIN: AMOUNT OF RAINFALL
C                   UMW: WET REMOVAL RATE OF WATER (NET CONDENSATION)
C OUTPUT VIA COMMON: C: CONCENTRATION PROFILES OF H2O(G) AND WATER
C                   RN: WET REMOVAL COEFFICIENTS
```

SUBROUTINE WETRM (TROPO)

```
IMPLICIT REAL*8 (A-H,O-Z)
```

```
COMMON-REGIONS
```

```
COMMON /ISWTCH/ IP(12)
COMMON /CONC/   C1(0:99,0:33),C2(0:99,1:30)
COMMON /MET    / EDD(0:99),TEMP(0:99),DZ
COMMON /RAIN   / PHW,PVULK(0:99),PLIGHT(0:99),PSST(0:99),PRB(0:99)
COMMON /RATEAK/ R(200,0:99),D(70,0:99),RN(20,0:99)
COMMON /RATE   / RR(200,0:99),DD(11,70,0:99),RNN(20,0:99),
*              AVK(200,2),NEP(300,6)
```

```
DECLARATIONS
```

```
REAL *8 AM (0:99), H2O (0:99), WSSR(0:99), TEXT (4), UMW (0:99),
1      PDAMPF(2),L(2),A(2), RAIN(0:99), ANH3(0:99),SO2(0:99),
2      FEUCHT(0:20)
INTEGER*4 NX(6),NEP
```

```
EQUIVALENCE
```

```

EQUIVALENCE (AM(0),C1(0,0)),(H2O(0),C1(0,16)),(WSSR(0),C1(0,17)),
1      (ANH3(0),C1(0,12)),(SO2(0),C2(0,15))
FKT(I)=1./(EXP(2.*(I-7.))+1.)
HKT(I)=.121*EXP(.256*(I)-.0436*(I)**2)
DATA FEUCHT /70.,58.,60.,60.,55.,45.,33.,29.,26.,24.,
1      22.,21.,21.,21.,21.,21.,19.5,12.1,7.4,4.13,2.6/
CALL MASKE

```

C
C
C
C

CALCULATION OF WATER VAPOR

```

RAINFK=IP(1)
L(1)=2500*18
L(2)=2834*18
A(1)=-2.274*18
A(2)=-0.14*18
T0=273
P0=610.78/101325
RB=8.314
DO 19 I=0,20
  DO 18 J=1,2
    PDAMPF(J)=P0*DEXP((L(J)-A(J)*T0)/RB*(1/T0-1/TEMP(I))+
*      A(J)/RB*DLOG(TEMP(I)/T0))
18  CONTINUE
    H2O(I)=FEUCHT(I)/100.*(PDAMPF(1)*FKT(I)
*      +PDAMPF(2)*(1.-FKT(I)))*AM(1)
19  CONTINUE
    DO 24 I=1,20
      IF (H2O(I)/AM(I).GT.H2O(I-1)/AM(I-1)) GOTO 25
24  CONTINUE
25  I0=I-1
    X1=DLOG(H2O(I0)/AM(I0))
    X2=DLOG(4.D-06)
    DO 29 I=I0,20
      H2O(I)=DEXP(X1+(X2-X1)/(21-I0)*(I-I0))*AM(I)
29  CONTINUE

```

C
C
C
C

CALCULATION OF WET REMOVAL

```

PHI0=-1.E+17
X=SQRT(EDD(2)*AM(2)*EDD(1)*AM(1))*(H2O(2)/AM(2)-H2O(1)/AM(1))/DZ
PHI0=2.*PHI0-X
DO 39 I=0,19
  PHI=SQRT(EDD(I+1)*AM(I+1)*EDD(I)*AM(I))*(H2O(I+1)/AM(I+1)-
*      H2O(I)/AM(I))/DZ
  UMW(I)=(PHI-PHI0)/DZ
  RAIN(I)=(PHI+PHI0)/2.
  PHI0=PHI
39  CONTINUE
  UMW(20)=0.
  RAIN(20)=RAIN(19)

```

C

```

IS=4
WRITE (11) IS
WRITE (11) UMW
WRITE (11) RAIN

```

C
C
C
C

CALCULATION OF LIQUID WATER

```

VRAIN=-50.
ITROPO=TROPO

```

```

Q0=(EDD(2)*AM(2)+EDD(1)*AM(1))/(ANH3(2)/AM(2)-ANH3(1)/AM(1))
DO 69 I=0,20
  WSSR(I)=RAIN(I)/VRAIN/(EXP((I-ITROPO)*1.5)+1.)
  RNTX=DMAX1(0.DO,UMW(I)/H2O(I))
  R1=WSSR(I)/HKT(I)
  RN(1,I)=(RNN(8,I)/(1.+RNN(8,I)*R1)*UMW(I))*RAINFK
  XW=RNN(10,I)/PHW
  RN(2,I)=(XW/(1.+XW*R1)*UMW(I)*FKT(I))*RAINFK
  RN(3,I)=1.*RNTX*RAINFK
  Q1=(EDD(I+1)*AM(I+1)+EDD(I)*AM(I))/(ANH3(I+1)/AM(I+1)-
1    ANH3(I)/AM(I))
C  PNNH4(I)=((Q1-Q0)/(2.*DZ*DZ)+PNH3(I)-DNH3(I)*ANH3(I))*RAINFK
  Q0=Q1
  SLHCL=3.
  RN(5,I)=SLHCL*RNTX*RAINFK
  XW=RNN(1,I)*(1.+RNN(2,I)/PHW*(1.+RNN(3,I)/PHW))
  DNSO2=(XW/(1.+XW*R1)*UMW(I)*FKT(I))*RAINFK
  RN(7,I)=(RNN(5,I)/(1.+RNN(5,I)*R1)*UMW(I))*RAINFK
  SO3ION=RNN(1,I)*RNN(2,I)/PHW*RNN(3,I)/PHW/(1+XW*R1)*XW*FKT(I)
  PNH3O=(RNN(4,I)*SO3ION*SO2(I)*HKT(I))*RAINFK
  RN(6,I)=DNSO2+RNN(4,I)*SO3ION*HKT(I)*RAINFK
  RN(8,I)=(RNN(11,I)/(1.+RNN(11,I)*R1)*UMW(I)*FKT(I))*RAINFK
  RN(9,I)=SLHCL*RNTX*RAINFK
  SLCH2O=1.
  RN(10,I)=SLCH2O*RNTX*RAINFK
69 CONTINUE
C
  READ (10,2000) NR,TEXT
  WRITE (6,2100) TEXT
  DO 79 J=1,NR
    READ (10,2200) J1,NX,TEXT
    WRITE (6,2300) J1,RN(J1,3),NX,TEXT
    DO 79 I=1,6
      NEP(270+J1,I)=NX(I)
79 CONTINUE
C
2000 FORMAT (I3,4A8)
2100 FORMAT ('1',4A8)
2200 FORMAT (I3,28X,2(I2,1X),A1,3(1X,I2),4A8)
2300 FORMAT (' ',I3,35X,1P,E10.2,4X,2I3,A2,3I3,3X,4A8)
  RETURN
  END
/*

```

```
//ICH301C1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C1,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          CCC      1
C          C        1 1
C          C        1
C          CCC      1
```

```
C *****
C *
C *      SUBROUTINE CALCULATION OF PHOTODISSOCIATION MATRIX      *
C *
C *****
```

```
C PURPOSE          : CALCULATION OF THE PHOTODISSOCIATION FREQUENCIES
C                   FOR FIXED ZENITH ANGLES FROM 89 DEGREE TO
C                   OVERHEAD SUN
C INPUT VIA COMMON : AM          : AIR DENSITY
C                   O3           : OZONE CONCENTRATION
C                   ANO2          : CONCENTRATION OF NO2
C                   VO2,DVO2      : COLUMN DENSITY OF OXYGEN
C                   VM,DVM        : COLUMN DENSITY OF AIR
C OUTPUT VIA COMMON: DD          : MATRIX OF PHOTODISSOCIATION FREQUENCIES
C OUTPUT ON PRINTER: PHOTON FLUXES AT DIFFERENT ZENITH ANGLES
C                   PHOTODISSOCIATION FREQUENCIES FOR OVERHEAD SUN
```

```
C      SUBROUTINE DISMAT
```

```
C      IMPLICIT REAL*8 (A-H,O-Z)
```

```
C      COMMON-BEREICHE
```

```
C      -----
C      COMMON /CONC/   C1(0:99,0:33),C2(0:99,1:30)
C      COMMON /SPECT/  WAVE(130),FLUX(130),S(70,130),ABSS(7,130),
C      *              RED(8,9),STF(8,70),SUBST(70)
C      COMMON /RATE/   R(200,0:99),DD(11,70,0:99),RN(20,0:99),
C      *              AVK(200,2),NEP(300,6)
C      COMMON /RATEAK/  RA(200,0:99),DA(70,0:99),RNA(20,0:99)
C      COMMON /SL/      VO2(0:99), VO3(0:99), VNO2(0:99), VM(0:99),
C      *              DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
C      COMMON /ZENITH/  ALPHA,BETA,TAU(0:99)
```

```
C      DIMENSIONS
```

```
C      -----
C      DIMENSION D(70,0:99),AM(0:99),O3(0:99),ANO2(0:99),
C      1          FOUT(130,7),FTOT(0:99)
```

```
C      EQUIVALENCE
```

```
C      -----
C      EQUIVALENCE (AM(0),C1(0,0)),(O3(0),C2(0,3)),(ANO2(0),C2(0,6))
```

```
C      IEND=99
```

```
C      JEND=40
```

```
C      DZ=1.E+05
```

```
C      PI=3.1415927
```

```
C      CALCULATION OF PHOTODISSOCIATION RATES
```

```
C      -----
```

```
Z0=DARCOS(ALPHA+BETA)*180./PI
CALL SAEUL (DZ,O3,VO3,DVO3)
CALL SAEUL (DZ,ANO2,VNO2,DVNO2)
IS=40
WRITE(11) IS
DO 99 NH=1,10
  RNH=NH
  RNH=(RNH-1.)/(10.-1.)
  ZENIT=Z0+(97.-Z0)*DCOS(RNH/2.*PI)
  WRITE (6,2140) ZENIT
  DO 91 L=1,130
    CALL BEAM (L,FTOT,ZENIT)
    ITP=1
    CALL PHOTO (ITP,FTOT,L,AM,D)
    DO 90 I=0,60,10
      IX=I/10+1
      FOUT(L,IX)=FTOT(I)
90    CONTINUE
    WRITE (6,2150) WAVE(L),(FTOT(I),I=0,60,10),FLUX(L)
91    CONTINUE
    WRITE (11) ZENIT
    WRITE (11) FOUT
    DO 95 J=1,JEND
      DO 95 I=0,IEND
        DD(NH,J,I)=D(J,I)
95    CONTINUE
    IF (ZENIT.LT.90.DO) THEN
      DO 96 I=0,IEND
        Z4=I**4
        A=0.2+5.3*DEXP(-2.09D-6*Z4)
        FAK=0.06+0.32*(1.DO-DEXP(-8.56D-7*Z4))
        DD(NH,4,I)=D(4,I)/FAK*DEXP(-A*(1./DCOS(ZENIT*PI/180.)-1.))
96    CONTINUE
      ELSE
        DO 97 I=0,IEND
97    DD(NH,4,I)=0.DO
      END IF
99 CONTINUE
C
C   OUTPUT OF NOON DATA
C   -----
  N1=1
  N=10
  DO 109 L=1,JEND/10
    WRITE (6,2010) ((J),J=N1,N),(SUBST(J),J=N1,N)
    WRITE (6,2020) (I,(D(J,I),J=N1,N),I=0,IEND,2)
    N1=N+1
    N=N+10
109 CONTINUE
C
  IF (PI.NE.0.) RETURN
  DO 119 J=1,JEND
    WRITE (6,2030) J,SUBST(J)
    DO 119 NH=1,10
      WRITE (6,2020) NH,(DD(NH,J,I),I=1,50,5)
119 CONTINUE
C
C   CALCULATION OF AVERAGING FACTOR      (NOT ACTIVE)
C   -----
  IF (PI.NE.0.) RETURN
  DO 219 NH=1,6
    TIME=11.5+NH
    CALL DAKT (TIME,6.,IEND)
```

```

      DO 209 J=1,40
        DO 209 I=0,IEND
          DD(11,J,I)=DD(11,J,I)+DA(J,I)
209   CONTINUE
219 CONTINUE
      TIME=12.
      CALL DAKT (TIME,6.,IEND)
      DO 229 J=1,40
        DO 229 I=0,IEND
          IF (DA(J,I).EQ.0.) GOTO 229
          DD(11,J,I)=(DD(11,J,I)/24.)/DA(J,I)
229 CONTINUE
      RETURN
C      FORMATS
C      -----
C
2010 FORMAT ('1',39X,'PHOTODISSOCIATIONS-COEFFICIENT IN S-1 FOR OVERHEA
      *D SUN'//' ALT',6X,10(I2,10X)/11X,10(A8,4X)/)
2020 FORMAT (I5,1P,10E12.2)
2030 FORMAT (///I10,10X,A8)
2140 FORMAT ('1 PHOTON-FLUXES',10X,'ZENITH-ANGLE ',F8.2//
      *      /'0 WAVE !    0 KM    !    10 KM    !    20 KM
      *      !    30 KM    !    40 KM    !    50 KM    !    60 KM    !',
      *      ' 100 KM    !'/113('='))
2150 FORMAT (' ',F7.1,' ! ',8(1P,E10.3,' ! '))
      END
/*

```

```
//ICH301C2 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C2,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C
C          CCC      22
C          C        2
C          C        2
C          CCC      2222
C
C *****
C *
C *      UNTERPROGRAMM: CALCULATION OF COLUMN DENSITIES *
C *
C *****
C
C PURPOSE          : CALCULATION OF THE COLUMN DENSITY OF
C                   A COMPONENT OF THE AIR
C INPUT VIA CALL   : DZ: ALTITUDINAL SPACING
C                   X: CONCENTRATION PROFILE OF THE COMPOUND
C OUTPUT VIA CALL  : Y: COLUMN DENSITY OF THE COMPOUND
C                   Z: DIFFERENTIAL COLUMN DENSITY
C
C      SUBROUTINE SAEUL (DZ,X,Y,Z)
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C      DIMENSION X(0:99),Y(0:99),Z(0:99)
C
C      SCALEHEIGHT
C      -----
C      IEND=99
C      SH=20./DLOG(X(IEND-20)/X(IEND))*DZ
C
C      COLUMN DENSITY
C      -----
C      Y(IEND)=X(IEND)*SH
C      Z(IEND)=Y(IEND)
C      DO 9 I=IEND-1,0,-1
C      IF (X(I).EQ.X(I+1)) GOTO 8
C      A=DZ/DLOG(X(I+1)/X(I))
C      Y(I)=Y(I+1)+A*(X(I+1)-X(I))
C      Z(I)=A*(DSQRT(X(I+1)*X(I))-X(I))
C      Z(I+1)=Z(I+1)+A*(X(I+1)-DSQRT(X(I+1)*X(I)))
C      GOTO 9
C 8 Y(I)=Y(I+1)+X(I)*DZ
C   Z(I)=X(I)*DZ/2.
C   Z(I+1)=Z(I+1)+X(I)*DZ/2.
C 9 CONTINUE
C
C 100 RETURN
C   END
/*
```

//ICH301C3 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)

/*PASSWORD MODEL

/*ROUTE PRINT MVS

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C3,

// PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K

//C.SYSIN DD *

```

C
C          CCC      333
C          C        -3
C          C        -3
C          CCC      333

```

```

C *****
C *                                     *
C *   UNTERPROGRAMM: CALCULATION OF PHOTON-FLUXES   *
C *                                     *
C *****

```

```

C PURPOSE          : CALCULATION OF THE PHOTON FLUX AT A GIVEN
C                   WAVELENGTH FOR THE ALTITUDINAL RANGE FROM
C                   GROUND TO 100KM. INCLUDED IS ABSORPTION BY
C                   O2,O3,NO2, AND RAYLEIGH SCATTERING AND
C                   GROUND AND CLOUD ALBEDO.
C INPUT VIA CALL    : WEG: COS(ZENITH ANGLE)
C                   L: INDEX OF THE WAVELENGTH INTERVALL
C INPUT VIA COMMON  : FLUX: EXTRATERRISTIC PHOTON FLUX
C                   ABSS: ABSORPTION CROSS-SECTIONS
C                   R: COEFFICIENTS FOR ABSORPTION IN THE
C                     SCHUMANN-RUNGE BANDS
C                   VX: INTEGRATED COLUMN DENSITY OF SPECIES X
C                   DVX: DIFFERENTIAL COLUMN DENSITY
C                   IRAIN: SWITCH    =0 NO CLOUDS
C                               =1 WITH CLOUD ALBEDO
C OUTPUT VIA CALL   : FTOT: ALTITUDINAL DEPENDENT PHOTON FLUX AT A
C                   GIVEN WAVELENGTH INTERVALL

```

SUBROUTINE STRAHL (WEG,L,FTOT,ZENIT)

DECLARATIONS

IMPLICIT REAL*8 (A-H,O-Z)

COMMON-REGIONS

```

COMMON/SPECT/  WAVE(130),FLUX(130),S(70,130),ABSS(7,130),R(8,9),
*              STF(8,70),SUBST(70)
COMMON/SL/     VO2(0:99),VO3(0:99),VNO2(0:99),VM(0:99),
*              DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
COMMON/ISWTCH/ IP(12)

```

DIMENSIONS

```

1  DIMENSION RTAUSR(0:99),FTOT(0:99),FU(0:99),FO(0:99),F(0:99),
      G(0:99)

```

FORMAT

88 FORMAT (I5,1P,12E10.3)

DATA

```
C      ----
C      DATA RTAUSR /100*1./
C
C      HKT(IX)=.121*EXP(.256*(IX)-.0436*(IX)**2)/2.*WALB
C      CALL MASKE
C
C      STREU=(ABSS(5,L)) *2.
C      PI=3.1415927
C      BALB=0.167
C      IRAIN=IP(1)
C      WALB=.7*IRAIN
C      IEND=99
C      IF (L.GT.9) GOTO 200
C
C      SCHUMANN-RUNGE BANDS
C
C      TAUSRO=1.
C      ABSS(1,L)=0.
C      DO 129 J=IEND-1,0,-1
C      DIFF=DLOG(VO2(J)/WEG*1.D-25)
C      RED=R(1,L)+R(2,L)*DIFF+R(3,L)*DIFF**2+R(4,L)*DIFF**3+
C      *      R(5,L)*DIFF**4+R(6,L)*DIFF**5+R(7,L)*DIFF**6+R(8,L)*DIFF**7
C      TAUSR=0.
C      IF (RED.LE.5)  TAUSR=DEXP(-DEXP(RED))
C      RTAUSR(J)=0.
C      IF (TAUSRO.NE.0.) RTAUSR(J)=TAUSR/TAUSRO
C      TAUSRO=TAUSR
129  CONTINUE
200  CONTINUE
C
C      UPPER BOUNDARY
C      -----
C      F (IEND)=DEXP(-(ABSS(1,L)*DVO2(IEND)+ABSS(2,L)*DVO3(IEND)+
C      *      ABSS(3,L)*DVNO2(IEND))/WEG)
C      G(IEND)=0.
C      FU(IEND)=FLUX(L)*F(IEND)
C
C      DO 217 J=IEND-1,70,-1
C      F(J)=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)
C      *      +ABSS(3,L)*DVNO2(J))/WEG)
C      G(J)=0.
C      FU(J)=FU(J+1)*RTAUSR(J)*F(J)
C      RTAUSR(J)=1.
217  CONTINUE
C      DO 218 J=69,20,-1
C      EXTAU=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)
C      *      +ABSS(3,L)*DVNO2(J))/WEG)
C      X=DEXP(-(ABSS(1,L)*(VO2(0)-VO2(J))+ABSS(2,L)*(VO3(0)-VO3(J))
C      *      +ABSS(3,L)*(VNO2(0)-VNO2(J)))/WEG)
C      EXTAUR=DEXP(-STREU*DVM(J)/WEG)
C      Y=DEXP(-STREU*(VM(0)-VM(J))/WEG)
C      F(J)=EXTAU*EXTAUR
C      FX=X*Y
C      G(J)=.5*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
C      GX=.5*(1.-Y)/(1.-X*(1.-Y))
C      FOX=BALB*(FX*(1.+GX))**2/(1.-FX*GX*BALB)+FX*GX
C      FU(J)=FU(J+1)*RTAUSR(J)*F(J)*(1.+G(J)+FOX*G(J))
C      RTAUSR(J)=1.
218  CONTINUE
C      DO 219 J=19,1,-1
C      EXTAU=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)
C      *      +ABSS(3,L)*DVNO2(J))/WEG)
C      X=DEXP(-(ABSS(1,L)*(VO2(0)-VO2(J))+ABSS(2,L)*(VO3(0)-VO3(J))
```

```

*      +ABSS(3,L)*(VNO2(0)-VNO2(J))/WEG)
EXTAUR=DEXP(-STREU*DVM(J)/WEG)+1.D-75
Y=DEXP(-STREU*(VM(0)-VM(J))/WEG)
F(J)=EXTAU*EXTAUR
FX=X*Y
G(J)=.5*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
GX=.5*(1.-Y)/(1.-X*(1.-Y))
FOX=BALB*(FX*(1.+GX))**2/(1.-FX*GX*BALB)+FX*GX
Y=6366./(6366.+J)
I=ZENIT/(PI/2.+DARCOS(Y))
Y=1-I
FU(J)=FU(J+1)*RTAUSR(J)*F(J)*(1.-HKT(J)+G(J)+FOX*G(J))*Y
RTAUSR(J)=1.

```

219 CONTINUE

C
C
C

LOWER BOUNDARY

```

EXTAU=DEXP(-(ABSS(1,L)*DVO2(0)+ABSS(2,L)*DVO3(0)
*      +ABSS(3,L)*DVNO2(0))/WEG)
EXTAUR=DEXP(-STREU*DVM(0)/WEG)
F(0)=EXTAU*EXTAUR
G(0)=.5*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
FU(0)=FU(1)*RTAUSR(0)*F(0)*(1.+G(0))/(1.-BALB*F(0)*G(0))
FO(0)=BALB*FU(0)*F(0)*(1.+G(0))+FU(1)*F(0)*G(0)
FTOT(0)=FU(0)*(1.+BALB)+(FU(1)+FU(0)*BALB)*4.*G(0)*(G(0)+1.)
RTAUSR(0)=1.

```

C
C
C

UPWARDS FLUX

```

DO 227 J=1,19
FO(J)=FO(J-1)*F(J)*(1.+G(J))+FU(J+1)*(G(J)+HKT(J))
FTOT(J)=SQRT(FU(J+1)*FU(J))+SQRT(FO(J-1)*FO(J))+
*      (FU(J+1)+FO(J-1))*4.*G(J)*(G(J)+1.)

```

227 CONTINUE

```

DO 228 J=20,69
FO(J)=FO(J-1)*F(J)*(1.+G(J))+FU(J+1)*G(J)
FTOT(J)=SQRT(FU(J+1)*FU(J))+SQRT(FO(J-1)*FO(J))+
*      (FU(J+1)+FO(J-1))*4.*G(J)*(G(J)+1.)

```

228 CONTINUE

```

DO 229 J=70,IEND-1
FO(J)=F(J)*FO(J-1)
FTOT(J)=SQRT(FU(J+1)*FU(J))+SQRT(FO(J-1)*FO(J))

```

229 CONTINUE

```

FO(IEND)=F(IEND)*FO(IEND-1)
FTOT(IEND)=FU(IEND)+FO(IEND)

```

C

RETURN
END

/*

```
//ICH301C4 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C4,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C          CCC  4  4
C          C    4  4
C          C    44444
C          CCC  4
C
C *****
C *                                     *
C *   UNTERPROGRAMM: PHOTODISSOCIATION FREQUENCIES   *
C *                                     *
C *****
C
C PURPOSE          : CALCULATION OF THE PHOTODISSOCIATION
C                   FREQUENCIES AT A GIVEN WAVELENGTH INTERVALL
C INPUT VIA CALL   : FL   : PHOTON FLUX AT THE WAVELENGTH INTERVALL
C                   L     : INDEX OF THE WAVELENGTH INTERVALL
C                   AM     : DENSITY OF AIR
C                   DA     : PHOTODISSOCIATION FREQUENCIES INTEGRATED
C                           UPTO WAVELENGTH (L+1)
C INPUT VIA COMMON : WAVE  : WAVELENGTH
C                   S     : ABSORPTION CROSS-SECTION
C                   STF    : COEFFICIENTS FOR THE TEMPERATURE DEPENDENCE
C                           OF THE ABSORPTION CROSS-SECTION
C                   LAMO,DLAM: COEFFICIENTS OF THE PRESSURE OR
C                           TEMPERATURE DEPENDENCE OF THE QUANTUM YIELD
C                   SLYM   : CROSS-SECTION AT LYMAN ALPHA LINE
C                   VO2    : COLUMN DENSITY OF OXYGEN
C                   T      : TEMPERATURE
C OUTPUT VIA CALL  : DA    : PHOTODISSOCIATION FREQUENCIES INTEGRATED
C                           UPTO WAVELENGTH L
C REMARKS          : THE PHOTODISSOCIATION REACTION WITH THE
C                   QUANTUM YIELD =1 FOR LONGER WAVELENGTHS
C                   MUST FOLLOW IMMEDIATELY THE REACTION WITH THE
C                   INVERSE QUANTUM YIELD
C
C   SUBROUTINE PHOTO (ITYP,FL,L,AM,DA)
C   =====
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C   COMMON
C   -----
C   COMMON / MET   / EDD(0:99),T(0:99),DZ
C   COMMON / SL    / VO2(0:99), VO3(0:99), VNO2(0:99), VM(0:99),
C   *              DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
C   COMMON /SPECT / WAVE(130),FLUX(130),S(70,130),ABSS(7,130),
C   *              R(8,9),STF(8,70),SUBSTZ(70)
C   COMMON /YIELD / LAMO(2,70),DLAM(2,70),SLYM(70),TFAK(0:99,70)
C
C   DIMENSION
C   -----
C   REAL *8 FL(0:99),DA(70,0:99),AM(0:99),QY2(0:99),LAMO
C   INTEGER *4 NRR(70)
C
C   DATA
C   ----
C   DATA NRR /0,40058,-40058,0,70075,92122,+92122,7*0,
```



```

*          14021,0,0,17024,1130,-1130,10*0,41080,-41080,38*0/
C
CALL MASKE
C
NRE=40
IEND=65
IF (ITYP.EQ.1) IEND=99
IF (L.NE.1) GOTO 20
DO 19 I=0,IEND
DO 18 NR=1,NRE
DA(NR,I)=1.5D+13*DEXP(-1.D-20*VO2(I))*SLYM(NR)
18 CONTINUE
DA(4,I)=4.55D-6*DEXP(-1.D-8*VO2(I)**(.38))
19 CONTINUE
20 CONTINUE
C
C
DO 99 NR=1,NRE
IF (S(NR,L).EQ.0.) GOTO 99
IF (STF(1,NR).EQ.0.) GOTO 30
DO 29 I=0,IEND
TFAK(I,NR)=1.-STF(1,NR)*(295.-T(I))**STF(2,NR)*DEXP(
1 STF(3,NR)*(WAVE(L)-1843.5)**2)*(WAVE(L)-1843.5)**STF(4,NR)
29 CONTINUE
30 CONTINUE
C
LE=ABS(NRR(NR))
LO=LE/1000
LE=LE-LO*1000
C BRANCHING
C
IF (NRR(NR)) 32,40,31
31 IF (L.GT.LE) GOTO 99
IF (L.LT.L0) GOTO 40
IF (NR.EQ.19) GOTO 60
GOTO 50
32 IF (L.GT.LE) GOTO 40
IF (L.LT.L0) GOTO 99
GOTO 65
C QUANTUM YIELD = 1
C
40 DO 49 I=0,IEND
DA(NR,I)=DA(NR,I)+S(NR,L)*FL(I)*TFAK(I,NR)
49 CONTINUE
GOTO 99
C CALCULATION OF QUANTUM YIELD
C
50 DO 59 I=0,IEND
WERT=(WAVE(L)-(LAM0(1,NR)+LAM0(2,NR)*T(I)))/
* (DLAM(1,NR)+DLAM(2,NR)*T(I))
QY=1./(DEXP(WERT)+1.)
QY2(I)=1.-QY
DA(NR,I)=DA(NR,I)+QY*S(NR,L)*FL(I)*TFAK(I,NR)
59 CONTINUE
GOTO 99
C PHOTOLYSIS FOR NR=19,20
C
60 DO 64 I=0,IEND
WERT=(WAVE(L)-(LAM0(1,19)+LAM0(2,19)/AM(I)))/
* (DLAM(1,19)+DLAM(2,19)/AM(I))
QY1=1./(DEXP(WERT)+1.)
WERT=(WAVE(L)-(LAM0(1,20)+LAM0(2,20)*T(I)))/
* (DLAM(1,20)+DLAM(2,20)*T(I))

```

```

      QY2(I)=0.83/DSQRT(DEXP(WERT)+1.)
      QY=QY1-QY2(I)
      DA(NR,I)=DA(NR,I)+QY*S(NR,L)*FL(I)*TFAK(I,NR)
64      CONTINUE
      GOTO 99
C      INVERSE QUANTUM YIELD
C      =====
65      DO 69 I=0,IEND
          DA(NR,I)=DA(NR,I)+QY2(I)*S(NR,L)*FL(I)*TFAK(I,NR)
69      CONTINUE
99      CONTINUE
C
      IF (L.NE.130) RETURN
      DO 109 I=0,IEND
          DA(28,I)=DA(27,I)*.01
          DA(7,I)=DMAX1(0.DO,(DA(7,I)-DA(6,I)))
109      CONTINUE
C
100      FORMAT (1P,12E10.2)
200      FORMAT (20I6)
      RETURN
      END
/*
```

```
//ICH301C5 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C5,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
C
C          CCC      5555
C          C        5
C          C        5  5
C          CCC      555
C
C *****
C *                                     *
C *   UNTERPROGRAMM: ACTUAL PHOTODISSOZIATION-FREQUENCIES   *
C *                                     *
C *****
C
C PURPOSE           : CALCULATION OF THE ACTUAL, INTERPOLATED PHOTO-
C                   DISSOCIATION FREQUENCIES AT 'TIME'
C INPUT VIA CALL    : TIME      : TIME FOR WHICH THE PHOTODISSOCIATION
C                   FREQUENCIES ARE REQUIRED
C                   SUNSET      : TIME OF SUNSET
C                   IDH          : ALTITUDINAL STEP
C INPUT VIA COMMON  : ALPHA,BETA: SIN*SIN AND COS*COS OF DECL,PHI
C                   DD          : MATRIX OF FIXED PHOTODISSOCIATION FREQUENCIES
C                   AS BUILT UP BY SUBPROGRAM DISMAT
C OUTPUT VIA COMMON : D          : ACTUAL PHOTODISSOCIATION FREQUENCIES
C REMARKS           : FROM SUNSET TO SUNRISE THE PHOTODISSOCIATION
C                   FREQUENCIES ARE SET EQUAL 0. DURING DAYTIME THE
C                   FREQUENCIES ARE INTERPOLATED LINEARLY BETWEEN THE
C                   TWO NEAREST VALUES OF MATRIX DD. INTERPOLATION
C                   PARAMETER IS THE ZENITH ANGLE.
C
C   SUBROUTINE DAKT (TIME,IDH,IEND)
C   =====
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C   COMMON
C   -----
C
C   COMMON /ZENITH/ ALPHA,BETA,TAU(0:99)
C   COMMON /RATEAK/ R(200,0:99),D(70,0:99),RN(20,0:99)
C   COMMON /RATE/  RR(200,0:99),DD(11,70,0:99),RRN(20,0:99),
C   *              AVK(200,2),NEP(300,6)
C
C   IANF=0
C   JEND=40
C   PI=3.1415927
C   DO 19 J=1,JEND
C       DO 19 I=IANF,IEND,IDH
C           D(J,I)=0.
C 19 CONTINUE
C
C   IF ((TIME.LE.6.DO).OR.(TIME.GE.18.DO)) RETURN
C
C   Z0=DARCOS(ALPHA+BETA)
C   Z1=97./180.*PI-Z0
C   ITM=TIME+6.
C   TM=ITM/12
C   TM=TM*12.
C   DO 29 I=IANF,IEND,IDH
```

```
TIM=(TIME-TM)*TAU(I)+TM
ZENIT=DARCOS(ALPHA+BETA*DCOS((TIM-12.)*PI/12.))
ZENIT=DMIN1(ZENIT,1.623D0)
I1=DARCOS((ZENIT-Z0)/Z1)*18./PI+1.
X=I1-1
I2=I1+1
ZEN1=Z0+Z1*DCOS(X/18.*PI)
ZEN2=Z0+Z1*DCOS((X+1.)/18.*PI)
DO 29 J=1,JEND
    D(J,I)=DD(I1,J,I)+(DD(I2,J,I)-DD(I1,J,I))/(ZEN2-ZEN1)*
*      (ZENIT-ZEN1)
29 CONTINUE
RETURN
100 FORMAT (1P,10E12.3)
END
/*
```

//ICH301C6 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)

/*PASSWORD MODEL

/*ROUTE PRINT MVS

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301C6,

// PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K

//C.SYSIN DD *

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      CCC      666
      C         6
      C         6  -6
      CCC      666

```

```

*****
*
*   UNTERPROGRAMM: CALCULATION OF PHOTON-FLUXES
*
*****

```

```

C PURPOSE          : CALCULATION OF THE PHOTON FLUX AT A GIVEN
C                   WAVELENGTH FOR THE ALTITUDINAL RANGE FROM
C                   GROUND TO 100KM. INCLUDED IS ABSORPTION BY
C                   O2,O3,NO2, AND RAYLEIGH SCATTERING AND
C                   GROUND AND CLOUD ALBEDO.
C INPUT VIA CALL   : WEG: COS(ZENITH ANGLE)
C                   L: INDEX OF THE WAVELENGTH INTERVALL
C INPUT VIA COMMON : FLUX: EXTRATERRISTIC PHOTON FLUX
C                   ABSS: ABSORPTION CROSS-SECTIONS
C                   R: COEFFICIENTS FOR ABSORPTION IN THE
C                     SCHUMANN-RUNGE BANDS
C                   VX: INTEGRATED COLUMN DENSITY OF SPECIES X
C                   DVX: DIFFERENTIAL COLUMN DENSITY
C                   IRAIN: SWITCH   =0 NO CLOUDS
C                             =1 WITH CLOUD ALBEDO
C OUTPUT VIA CALL  : FTOT: ALTITUDINAL DEPENDENT PHOTON FLUX AT A
C                   GIVEN WAVELENGTH INTERVALL

```

SUBROUTINE BEAM (L,FTOT,ZENIT)

DECLARATIONS

IMPLICIT REAL*8 (A-H,O-Z)

COMMON-REGIONS

```

COMMON/SPECT/  WAVE(130),FLUX(130),S(70,130),ABSS(7,130),R(8,9),
*              STF(8,70),SUBST(70)
COMMON/SL/     VO2(0:99),VO3(0:99),VNO2(0:99),VM(0:99),
*              DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
COMMON/ISWTCH/ IP(12)

```

DIMENSIONS

```

DIMENSION RTAUSR(0:99),FTOT(0:99),FU(0:99),FO(0:99),F(0:99),
1          G(0:99),WEG(0:99),JM(0:99),FAK(0:99)

```

FORMAT

```

77 FORMAT ('1  ACHTUNG !!! ',2I5,1P,E10.3,' !!! ACHTUNG'/////)
88 FORMAT (I5,1P,12E10.3)

```

DATA

```

C      ----
C      DATA RTAUSR /100*1./
C
C      HKT(IX)=.121*EXP(.256*(IX)-.0436*(IX)**2)/2.*WALB
C      CALL MASKE
C
C      STREU=ABSS(5,L)
C      PI=3.1415927
C      IRAIN=IP(1)
C      BALB=0.167
C      WALB=.7*IRAIN
C      RE=6366
C      IEND=99
C
C      CALCULATION OF ABSORPTION-LENGTH
C      -----
C      IF (L.GT.1) GOTO 110
C      PSI=DMAX1(ZENIT,90.D0)*PI/180.
C      SINPSI=DSIN(PSI)
C      SINZ=DSIN(ZENIT*PI/180.)
C      DO 109 I=0,IEND
C          RP=RE+I
C          X=RP*SINPSI-RE+.5
C          JM(I)=DMAX1(0.D0,X)
C          IF ((JM(I).GT.IEND).OR.(JM(I).LT.0)) WRITE (6,77) I,JM(I),X
C          FAK(I)=1.
C          IF (X.LT.0.D0) FAK(I)=0.
C          PHIO=DARSIN(RP*SINZ/((RP+1.)*SINPSI))
C          PHI1=DMIN1(PI-PHIO,ZENIT*PI/180.)
C          WEG(I)=RP*SINZ*(DCOTAN(PHIO)-DCOTAN(PHI1))
109  CONTINUE
110  CONTINUE
C
C      SCHUMANN-RUNGE BANDS
C      -----
C      IF (L.GT.9) GOTO 200
C      TAUSRO=1.
C      ABSS(1,L)=0.
C      DO 129 I=IEND-1,0,-1
C          DIFF=DLOG(VO2(I)*WEG(I)*1.D-25)
C          RED=R(1,L)+R(2,L)*DIFF+R(3,L)*DIFF**2+R(4,L)*DIFF**3+
C          * R(5,L)*DIFF**4+R(6,L)*DIFF**5+R(7,L)*DIFF**6+R(8,L)*DIFF**7
C          TAUSR=0.
C          IF (RED.LE.5) TAUSR=DEXP(-DEXP(RED))
C          RTAUSR(I)=0.
C          IF (TAUSRO.NE.0.) RTAUSR(I)=TAUSR/TAUSRO
C          TAUSRO=TAUSR
129  CONTINUE
200  CONTINUE
C
C      UPPER BOUNDARY
C      -----
C      J=JM(IEND)
C      F(IEND)=DEXP(-(ABSS(1,L)*VO2(J)+ABSS(2,L)*VO3(J)+
C      * ABSS(3,L)*VNO2(J))*WEG(IEND))*FAK(IEND)
C      G(IEND)=0.
C      FU(IEND)=FLUX(L)*F(IEND)
C
C      DOWNWARD FLUX
C      -----
C      DO 217 I=IEND-1,70,-1
C          J=JM(I)
C          F(I)=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)

```

```

*      +ABSS(3,L)*DVNO2(I))*WEG(J))*FAK(I)
G(I)=0.
FU(I)=FU(I+1)*RTAUSR(I)*F(I)
C      WRITE (6,88) I,WEG(I),FAK(I),F(I),G(I),FU(I)
      RTAUSR(I)=1.
217 CONTINUE
      DO 218 I=69,20,-1
      J=JM(I)
      EXTAU=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)
*      +ABSS(3,L)*DVNO2(J))*WEG(I))*FAK(I)
      X=DEXP(-(ABSS(1,L)*(VO2(0)-VO2(J))+ABSS(2,L)*(VO3(0)-VO3(J))
*      +ABSS(3,L)*(VNO2(0)-VNO2(J)))*WEG(I))*FAK(I)
      EXTAUR=DEXP(-STREU*DVM(J)*WEG(I))*FAK(I)
      Y=DEXP(-STREU*(VM(0)-VM(J))*WEG(I))*FAK(I)
      F(I)=EXTAU*EXTAUR
      FX=X*Y
      G(I)=.5*EXTAU*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
      GX=.5*(1.-Y)*X/(1.-X*(1.-Y))
      FOX=BALB*(FX+FX*GX)**2/(1.-BALB*FX*GX)+FX*GX
      FU(I)=FU(I+1)*RTAUSR(I)*F(I)*(1.+G(I)+FOX*G(I))
C      WRITE (6,88) I,WEG(I),FAK(I),F(I),G(I),FU(I),FX,GX,FOX,EXTAU
      RTAUSR(I)=1.
218 CONTINUE
      DO 219 I=19,1,-1
      J=JM(I)
      EXTAU=DEXP(-(ABSS(1,L)*DVO2(J)+ABSS(2,L)*DVO3(J)
*      +ABSS(3,L)*DVNO2(J))*WEG(I))*FAK(I)
      X=DEXP(-(ABSS(1,L)*(VO2(0)-VO2(J))+ABSS(2,L)*(VO3(0)-VO3(J))
*      +ABSS(3,L)*(VNO2(0)-VNO2(J)))*WEG(I))*FAK(I)
      EXTAUR=DEXP(-STREU*DVM(J)*WEG(I))*FAK(I)
      Y=DEXP(-STREU*(VM(0)-VM(J))*WEG(I))*FAK(I)
      F(I)=EXTAU*EXTAUR
      FX=X*Y
      G(I)=.5*EXTAU*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
      GX=.5*(1.-Y)*X/(1.-X*(1.-Y))
      FOX=BALB*(FX+FX*GX)**2/(1.-BALB*FX*GX)+FX*GX
      FU(I)=FU(I+1)*RTAUSR(I)*F(I)*(1.-HKT(I)+G(I)+FOX*G(I))
C      WRITE (6,88) I,WEG(I),FAK(I),F(I),G(I),FU(I),FX,GX,FOX,EXTAU
      RTAUSR(I)=1.
219 CONTINUE
C
C      LOWER BOUNDARY
C      -----
      EXTAU=DEXP(-(ABSS(1,L)*DVO2(0)+ABSS(2,L)*DVO3(0)
*      +ABSS(3,L)*DVNO2(0))*WEG(0))*FAK(0)
      EXTAUR=DEXP(-STREU*DVM(0)*WEG(0))*FAK(0)
      F(0)=EXTAU*EXTAUR
      G(0)=.5*EXTAU*(1.-EXTAUR)/(1.-EXTAU*(1.-EXTAUR))
      X=BALB*G(0)*F(0)
      FU(0)=FU(1)*RTAUSR(0)*F(0)*(1.+G(0))/(1.-X)
      FO(0)=BALB*FU(0)*F(0)*(1.+G(0))+FU(1)*F(0)*G(0)
      FTOT(0)=FU(0)*(1.+BALB)
C      WRITE (6,88) I,WEG(0),FAK(0),F(0),G(0),FU(0),FO(0),FTOT(0),EXTA
      RTAUSR(0)=1.
C
C      UPWARD FLUX
C      -----
      DO 227 I=1,19
      FO(I)=FO(I-1)*F(I)*(1.+G(I))+FU(I+1)*(G(I)+HKT(I))*F(I)
      FTOT(I)=SQRT(FU(I+1)*FU(I))+SQRT(FO(I-1)*FO(I))+
*      (FU(I+1)+FO(I-1))*2.*G(I)
227 CONTINUE
      DO 228 I=20,69

```

```
FO(I)=FO(I-1)*F(I)*(1.+G(I))+FU(I+1)*F(I)*G(I)
FTOT(I)=SQRT(FU(I+1)*FU(I))+SQRT(FO(I-1)*FO(I))+
*      (FU(I+1)+FO(I-1))*2.*G(I)
228 CONTINUE
DO 229 I=70,IEND-1
FO(I)=F(I)*FO(I-1)
FTOT(I)=SQRT(FU(I+1)*FU(I))+SQRT(FO(I-1)*FO(I))
229 CONTINUE
FO(IEND)=F(IEND)*FO(IEND-1)
FTOT(IEND)=FU(IEND)+FO(IEND)
C
RETURN
END
/* EOJ
```

```
//ICH301D1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D1,
//      PARM.C='MAP,XREF,OPTIMIZE(2),NOSDUMP',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          DDD          1
C          D  D        1 1
C          D  D          1
C          DDD          1
C
```

```
C *****
C *
C *   UNTERPROGRAMM :    STEADY-STATE VERSION   *
C *
C *****
```

```
C PURPOSE:          CALCULATION OF THE CONCENTRATION PROFILES OF THE
C                   AIR'S COMPONENTS UNDER STEADY-STATE CONDITIONS
C INPUT VIA CALL   : ITEND: NUMBER OF ITERATIONS
C INPUT VIA COMMON : C : CONCENTRATION PROFILES OF AIR,O3,NO2
C                   PC,DC : PRODUCTION RATES AND DESTRUCT. FREQUENCIES
C                   EX: COEFFICIENT OF THE BOUNDARY CONDITION
C                   WAVE : WAVELENGTHS OF SPECTRAL DATA
C                   FLUX : EXTRATERRISTIC PHOTONFLUX
C                   ALPHA,BETA : SIN*SIN AND COS*COS OF PHI,DECL
C                   EDD : EDDY-DIFFUSION COEFFICIENT
C                   DZ  : ALTITUDINAL SPACING
C                   RR  : GASPHASE REACTION COEFFICIENTS
C                   DD(11,,) : DIURNAL AVERAGING FACTOR OF PHOTO-
C                             DISSOCIATION FREQUENCIES
C                   AVK : COEFFICIENTS OF THE AVERAGING FACTORS OF
C                             GASPHASE REACTIONS
C                   IRATE: SWITCH  =0: NO OUTPUT OF INDIVIDUAL RATES
C                             =N: OUTPUT OF INDIVIDUAL RATES
C                             AT THE N.TH ITERATION
C                             N<0: ONLY OUTPUT OF THE REACTION-
C                                   NUMBER AND -SYMBOL
C                   INTOUT : SWITCH  =0: NO OUTPUT OF INTERM. PROFILES
C                             =1: OUTPUT OF INTERMEDIATE PROFILES
C                   ISUB : NUMBER OF COMPOUND NOT TO BE CALCULATED
C OUTPUT VIA COMMON: C : CONCENTRATION PROFILES
C                   R : DIURNALLY AVERAGED GASPHASE REACTION CONSTANTS
C                   D : DIURNALLY AVERAGED PHOTODISS. FREQUENCIES
C OUTPUT ON PRINTER: FTOT: PHOTONFLUXES FOR NOON CONDITIONS
C                   D : DIURNALLY AVERAGED PHOTODISS. FREQUENCIES
C
```

SUBROUTINE STEADY (ITEND)

```
C
C=====
```

IMPLICIT REAL*8 (A-H,O-Z)

```
C -----
```

COMMON-REGIONS

```
C -----
```

```
COMMON /ISWTC / IP(12)
COMMON /CONC/   C1(0:99,0:33),C2(0:99,1:30)
COMMON /TERME/  PC1(0:99,2:33), PC2(0:99,1:30),
*              DC1(0:99,2:33), DC2(0:99,1:30), TT(0:99,2:33)
COMMON /ZENITH/ ALPHA,BETA,TAU(0:99)
COMMON /MET     / EDD(0:99),TEMP(0:99),DZ
COMMON /SL      / VO2(0:99),VO3(0:99),VNO2(0:99),VM(0:99),
```

```
*          DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
COMMON /RATEAK / R(200,0:99),D(70,0:99),RN(20,0:99)
COMMON /RATE   / RR(200,0:99),DD(11,70,0:99),RRN(20,0:99),
*          AVK(200,2),NEP(300,6)
```

DIMENSIONS

```
-----
REAL *8 AM (0:99), ANO2(0:99), O3 (0:99), XALT (0:99,8),
*      XX(0:99), ZZ(0:99), PX(0:99), DX(0:99), XM(0:99),
*      FTOT(0:99),FTOT1(7,130)
INTEGER *4 NSUM(7),NEP,NFAM(10,7)
```

EQUIVALENCE

```
-----
EQUIVALENCE (AM(0),C1(0,0)),(O3(0),C2(0,3)),(ANO2(0),C2(0,6))
```

DATA

```
-----
DATA NSUM /3,8,6,2,2,5,5/
DATA NFAM /1,2,3,7*0,
1      4,5,6,7,8,9,10,22,2*0,
2      9,10,11,12,13,21,4*0,
3      14,15,8*0,
4      16,17,8*0,
5      18,19,20,21,22,5*0,
6      23,24,25,26,27,5*0  /
```

```
PI=3.1415927
INTOUT=IP(2)
IRATE=IP(3)
ISUB=IP(4)
IA=0
JF=0
IDH=1
IEND=99
JEND=40
ITYP=1
ISW=0
IF (IRATE.LT.0) ISW=1
IRATE=IABS(IRATE)
DO 29 J=1,200
  A=AVK(J,1)
  B=AVK(J,2)
  DO 28 I=0,60
    FAK=DMAX1(A+B*I,1.D-3)
    R(J,I)=RR(J,I)*FAK
28  CONTINUE
  DO 29 I=61,IEND
    R(J,I)=RR(J,I)*FAK
29  CONTINUE
```

ITERATIONS

```
=====
DO 39 IT=1,ITEND
  IF (IT.NE.2**JF) GOTO 301
  JF=JF+1
```

CALCULATION OF THE PHOTON FLUX AND PHOTOLYSIS RATES

```
-----
CALL SAEUL (DZ,O3,VO3,DVO3)
CALL SAEUL (DZ,ANO2,VNO2,DVNO2)
ZENIT=DARCOS(ALPHA+BETA)
```

```

WEG=ALPHA+BETA
IF (IT.GT.ITEND/2) THEN
  DO 38 L=1,130
    CALL STRAHL (WEG,L,FTOT,ZENIT)
    K2=0
    DO 37 K1=0,60,10
      K2=K2+1
      FTOT1(K2,L)=FTOT(K1)
37      CONTINUE
    CALL PHOTO (ITYP,FTOT,L,AM,D)
38    CONTINUE
    IS=6
    WRITE(11) IS
    WRITE(11) FTOT1
  ELSE
    DO 36 L=1,130
      CALL STRAHL (WEG,L,FTOT,ZENIT)
      CALL PHOTO (ITYP,FTOT,L,AM,D)
36    CONTINUE
  ENDIF
C
C  AVERAGING OVER ZENITHANGLE
C  -----
DO 35 J=1,JEND
  DO 35 I=0,IEND
    D(J,I)=D(J,I)*DD(11,J,I)
35  CONTINUE
  IF (IT.LE.ITEND/2) GOTO 301
  IS=7
  WRITE(11) IS
  WRITE(11) D
301 CONTINUE
C
C  CALCULATION OF THE PRODUCTION AND DESTRUCTION PROFILES
C  -----
CALL CHEMIE (IDH,IEND,ITYP)
CALL SMXRT
IF (IT.EQ.IRATE) CALL RATES(ISW)
C
C  CALCULATION OF THE TRANSPORT
C  -----
NSED=0.
DO 34 J=2,33
  IF ((J.EQ.17).OR.(J.EQ.ISUB)) GOTO 34
  IF (J.GT.8) GOTO 303
  DO 33 I=0,IEND
    XALT(I,J)=C1(I,J)
33    CONTINUE
303  CONTINUE
  IANF=0
  IF (J.EQ.16) IANF=20
  CALL GAUSS (IANF,IEND,J,NSED,XM)
  DO 34 I=IANF,IEND
    C1(I,J)=(XM(I)*AM(I)+C1(I,J))/2.
34  CONTINUE
C
C  CALCULATION OF THE NEW CONCENTRATIONS
C  -----
DO 320 J=2,8
  IF (J.EQ.ISUB) GOTO 320
  DO 32 K=1,NSUM(J-1)
    KX=NFAM(K,J-1)
    DO 32 I=0,IEND

```

```

32          C2(I,KX)=C2(I,KX)/XALT(I,J)*C1(I,J)
320  CONTINUE
C
C      INTERMEDIATE OUTPUT
C      -----
      IF (INTOUT.EQ.0) GOTO 39
      IF (IT.NE.2**IA) GOTO 39
          IA=IA+1
          IS=80+IA
          WRITE(11) IS
          WRITE(11) C1
          WRITE(11) C2
          RIT=IT
          IS2=2
          CALL OUTPT (RIT,IS2,IDH,IEND,ITYP)
39  CONTINUE
C
      IS=80
      WRITE(11) IS
      WRITE(11) C1
      WRITE(11) C2
      RITEND=ITEND
      IS1=1
      IS9=9
      CALL OUTPT (RITEND,IS1,IDH,IEND,IS9)
      CALL SAEUL (DZ,03,VO3,DVO3)
      WRITE (6,2250) ((I,VO3(I)),I=0,IEND)
      IDOB=VO3(0)/2.687D16
      WRITE (6,2200) IDOB
C
C      FORMATS
C      -----
2010  FORMAT (10I5)
2020  FORMAT (1P,10E12.2)
2030  FORMAT (I5,1P,10E12.2)
2200  FORMAT (/'OCOLUMN-DENSITY IS EQUIVALENT TO',I7,' DOBSON UNITS')
2250  FORMAT ('1 COLUMN-DENSITY OF 03 : '/(5(I5,'KM:',1PE12.4,'/CM-2'))))
      RETURN
      END
/*
```

// ICH301D2 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)

/*PASSWORD MODEL

/*ROUTE PRINT MVS

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D2,

// PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K

//C.SYSIN DD *

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                DDD      222
                D  D      2  2
                D  D      2
                DDD      2222
*****
*
*   UNTERPROGRAMM :   LONG-TERM VARIATION
*
*****

```

```

C PURPOSE          : CALCULATION OF THE LONGTERM VARIATIONS OF THE
C                   CONCENTRATION PROFILES OF THE AIR'S COMPONENTS
C INPUT VIA CALL    : NJAHR: NUMBER OF YEARS TO BE CALCULATED
C INPUT VIA COMMON : C   : STARTING VALUES FOR THE CONCENTRATIONS
C                   RR   : REACTION RATES
C                   AVK   : COEFFICIENTS OF THE AVERAGING FACTOR
C                   ALPHA,BETA: SIN*SIN AND COS*COS OF DECL,PHI
C                   DZ    : ALTITUDINAL SPACING
C                   IP2   : SWITCH   =0: NO INTERMEDIATE OUTPUT
C                           =1: OUTPUT AT THE END OF EACH YEAR
C OUTPUT VIA COMMON: C   : NEW CONCENTRATIONS
C                   R     : AVERAGED REACTION RATES
C OUTPUT ON PRINTER: FTOT : PHOTONFLUX AT NOON
C                   D     : AVERAGED PHOTODISSOCIATION FREQUENCIES
C                   VO3   : COLUMN DENSITY OF OZONE

```

SUBROUTINE LONGTM (NJAHR)

IMPLICIT REAL*8 (A-H,O-Z)

COMMON-BEREICHE

```

COMMON /CONC/      C1(0:99,0:33),C2(0:99,1:30)
COMMON /ISWTCH/    IP(12)
COMMON /ZENITH/    ALPHA,BETA,TAU(0:99)
COMMON /MET        / EDD(0:99),TEMP(0:99),DZ
COMMON /SL         / VO2(0:99),VO3(0:99),VNO2(0:99),VM(0:99),
1                  DVO2(0:99),DVO3(0:99),DVNO2(0:99),DVM(0:99)
COMMON /RATEAK/    R(200,0:99),D(70,0:99),RN(20,0:99)
COMMON /RATE       / RR(200,0:99),DD(11,70,0:99),RRN(20,0:99),
1                  AVK(200,2),NEP(300,6)
COMMON /SPECT/     WAVE(130),FLUX(130),S(70,130),ABSS(7,130),RED(8,9)
1                  ,STF(8,70),SUBST(70)

```

DIMENSIONEN

```

REAL *8      XALT(0:99,8),AM(0:99), O3(0:99), ANO2(0:99),FTOT(0:99)
INTEGER *4   NSUM(7),NFAM(10,7)
EQUIVALENCE (AM(0),C1(0,0)),(O3(0),C2(0,3)),(ANO2(0),C2(0,6))

```

DATA

```
DATA NSUM /3,8,6,2,2,5,5/
DATA NFAM /1,2,3,7*0,
1      4,5,6,7,8,9,10,22,2*0,
2      9,10,11,12,13,21,4*0,
3      14,15,8*0,
4      16,17,8*0,
5      18,19,20,21,22,5*0,
6      23,24,25,26,27,5*0 /
```

C

```
PI=3.1415927
IDH=1
IANF=0
IEND=65
JEND=33
ITYP=2
INTOUT=IP(2)
NTIMST=365
DT=3600. *24. *365. /NTIMST
NTIMST=3
```

```
DO 19 J=1,200
  A=AVK(J,1)
  B=AVK(J,2)
  DO 18 I=0,60
    FAK=DMAX1(A+B*I,1.D-3)
    R(J,I)=RR(J,I)*FAK
    TAU(I)=1.
```

```
18 CONTINUE
19 CONTINUE
```

C

```
DO 29 I=61,IEND
  R(J,I)=RR(J,I)*FAK
  TAU(I)=1.
```

```
29 CONTINUE
IS=1
CALL EULER (DT,IDH,IEND,IS)
CALL TRANS (IS,IDH,IEND,DT)
```

C

C

C

C

C

TIME STEPS

```
DO 39 IJ=1,NJAHR
```

C

C

C

CALCULATION OF PHOTODISSOCIATION

```
-----
CALL SAEUL (DZ,O3,VO3,DVO3)
CALL SAEUL (DZ,ANO2,VNO2,DVNO2)
IF ((IJ.EQ.1).OR.(IJ.EQ.NJAHR)) WRITE (6,2140)
ZENIT=DARCOS(ALPHA+BETA)
DO 37 L=1,130
  WEG=ALPHA+BETA
  CALL STRAHL (WEG,L,FTOT,ZENIT)
  IF ((IJ.EQ.1).OR.(IJ.EQ.NJAHR))
    * WRITE (6,2150) WAVE(L),(FTOT(I),I=0,IEND,10),FLUX(L)
  CALL PHOTO (ITYP,FTOT,L,AM,D)
```

```
37 CONTINUE
```

C

C

C

INTEGRATION UEBER TAG

```
-----
DO 36 J=1,JEND
  DO 36 I=IANF,IEND,IDH
    D(J,I)=D(J,I)*DD(11,J,I)
```

```
36 CONTINUE
```

```

      IF ((IJ.NE.1).AND.(IJ.NE.NJAHR)) GOTO 301
      N1=1
      N=10
      DO 35 L=1,4
        WRITE (6,2010) ((J),J=N1,N),(SUBST(J),J=N1,N)
        WRITE (6,2020) (I,(D(J,I),J=N1,N),I=0,IEND,2)
        N1=N+1
        N=N+10
35      CONTINUE
301     CONTINUE
      IS=2
      CALL TRANS (IS,IDH,IEND,DT)
C
C      CALCULATION OF NEW CONCENTRATIONS
C      -----
      DO 34 IM=1,NTIMST
        IS=3
        CALL TRANS (IS,IDH,IEND,DT)
        DO 33 J=2,8
          DO 33 I=IANF,IEND,IDH
            XALT(I,J)=C1(I,J)
33      CONTINUE
        CALL CHEMIE (IDH,IEND,ITYP)
        IS=3
        CALL EULER (DT,IDH,IEND,IS)
C
C      CONCENTRATIONS WITHIN GROUPS
C      -----
      DO 32 J=2,8
        KE=NSUM(J-1)
        DO 32 K=1,KE
          KX=NFAM(K,J-1)
          DO 32 I=IANF,IEND,IDH
            C2(I,KX)=C2(I,KX)*C1(I,J)/XALT(I,J)
32      CONTINUE
C
C      INTERMEDIATE OUTPUT
C      -----
      IF (INTOUT.EQ.0) GOTO 34
      RJ=IM
      CALL OUTPT (RJ,2,IDH,IEND,ITYP)
      WRITE (6,2000) IJ,IM
34      CONTINUE
C      CALL OUTLTM (IJ,IDH,1)
39      CONTINUE
C
      RJAHR=NJAHR
      CALL OUTPT (RJAHR,1,IDH,IEND,8)
C      CALL OUTLTM (NJAHR,IDH,2)
      CALL SAEUL (DZ,03,VO3,DVO3)
      WRITE (6,2250) ((I,VO3(I)),I=0,IEND)
C
C      FORMATE
C      -----
C
2000 FORMAT (10I5)
2010 FORMAT ('1',39X,'AVERAGED PHOTODISSOCIATION-COEFFICIENT IN S-1'
*          //' ALT+1',4X,10(I2,10X)/11X,10(A8,4X)/)
2020 FORMAT (I5,1P,10E12.2)
2140 FORMAT ('1 PHOTON-FLUXES FOR NOON CONDITIONS'//
*          /'0 WAVE      0 KM      10 KM      20 KM      30 KM
*          40 KM      50 KM      60 KM      100 KM'/113('='))
2150 FORMAT (F8.1,2X,8(1P,E10.3,3X))

```

- 4 -

```
2250 FORMAT ('1 COLUMN-DENSITY OF O3 : '/(5(I5,'KM:',1P,E12.4,'/CM-2')))  
      RETURN  
      END
```

/*

```
//ICH301D3 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D3,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C                      DDD      333
C                      D  D      _3
C                      D  D      _3
C                      DDD      333
C
```

```
C *****
C *
C *   UNTERPROGRAMM :   DIURNAL VARIATION
C *
C *****
```

```
C PURPOSE           : CALCULATION OF THE DIURNAL VARIATIONS OF
C                   : THE CONCENTRATION PROFILES
C INPUT VIA CALL    : NTAG: NUMBER OF DAYS TO BE CALCULATED
C                   : IDH : ALTITUDINAL STEP
C INPUT VIA COMMON : C   : STARTING VALUES OF THE CONCENTRATIONS
C                   : DZ  : ALTITUDINAL SPACING
C                   : ALPHA,BETA: SIN*SIN AND COS*COS OF DECL,PHI
C                   : RR   : REAKTION RATES
C                   : INTOUT : SWITCH   =0: NO INTERMEDIATE OUTPUT
C                   :                   =1: INTERMEDIATE OUTPUT
C                   : IMEAN:SWITCH =0: NO CALCULATION OF MEAN VALUES
C                   :                   =1: CALCUL. OF AVERAGING COEFFICIENTS
C OUTPUT VIA COMMON: C   : NEW CONCENTRATION PROFILES
C                   : R    : ACTUAL REAKTION RATES (=RR)
C                   : TAU  : TIME SHIFT FACTOR
C
```

```
      SUBROUTINE DIURNL (NTAG,IDH,IEND)
```

```
C
C=====
```

```
      IMPLICIT REAL*8 (A-H,O-Z)
```

```
      COMMON-REGIONS
```

```
C
C-----
C
```

```
      COMMON /TERME/  P1(0:99,2:33),P2(0:99,1:30),
*                   D1(0:99,2:33),D2(0:99,1:30),TT(0:99,2:33)
      COMMON /CONC/   C1(0:99,0:33),C2(0:99,1:30)
      COMMON /MET /    EDD(0:99),TEMP(0:99),DZ
      COMMON /ZENITH/  ALPHA,BETA,TAU(0:99)
      COMMON /RATEAK/  R(200,0:99),D(70,0:99),RN(20,0:99)
      COMMON /RATE /   RR(200,0:99),DD(11,70,0:99),RRN(20,0:99),
1      AVK(200,2),NEP(300,6)
      COMMON /ISWTCH/  IP(12)
```

```
C
C DIMENSIONS
C-----
```

```
      REAL *8      DTIME(20), XALT(0:99,8), TAUS(0:99), LTIME(0:99)
      INTEGER *4    NTIME(20), NSUM(7),NFAM(10,7)
```

```
C
C DATA
C-----
C
```

```
      DATA DTIME/900.,900.,300.,300.,180.,60.,20.,5.,20.,60.,300.,900.,
*          1800.,1800.,5.,20.,60.,180.,300.,300./
      DATA NTIME /8,8,12,12,25,30,39,24,45,45,24,12,6,6,24,39,30,25,12,
```

```

*          12/
DATA NSUM /3,8,6,2,2,5,5/
DATA NFAM /1,2,3,7*0,
1          4,5,6,7,8,9,10,22,2*0,
2          9,10,11,12,13,21,4*0,
3          14,15,8*0,
4          16,17,8*0,
5          18,19,20,21,22,5*0,
6          23, 24, 25, 26, 27, 5*0 /

```

C

```

PI=3.1415927
RERD=6.366E8
ITYP=3
ITS=15
IANF=0
INTOUT=IP(2)
IMEAN=IP(7)
IMIN=IP(10)
IMX=0
IF (IMIN.GT.0) IMX=1
TIME=10.
TV=TIME-.000001
TIMV=TV
TVM=TV+1.
THALF=2.
IS1=1
IS2=2
IS3=3
DO 19 I=0,IEND
  LTIME(I)=TIME
  Y=SQRT(1.-(RERD/(RERD+I*DZ))**2)+ALPHA
  X=2.
  IF (Y.LT.0.DO) X=0.
  IF (DABS(Y/BETA).LE.1.DO) X=DARCOS(-Y/BETA)/PI*2.
  X=DMAX1(X,0.DO)
  TAUS(I)=DMIN1(X,2.DO)
  TAU(I)=TAUS(I)
  DO 19 J=1,200
    R(J,I)=RR(J,I)

```

19 CONTINUE

C CALL TRANS (IS1,IDH,IEND,DT)

C

C

C

C

C

```

WRITE (6,2030)
DO 29 ID=1,NTAG
  IF (ID.EQ.NTAG) THALF=16.
  DO 28 IT=ITS,20
    IF (IT.NE.2) GOTO 210
    TIME=12.DO
    DO 209 I=0,IEND
      LTIME(I)=12.DO
209    CONTINUE
      DT=DTIME(IT)/THALF
      IF (IT.NE.9) GOTO 212
      DO 211 I=IANF,IEND
211    TAU(I)=2.-TAUS(I)
212    IF (IT.NE.15) GOTO 214
      DO 213 I=IANF,IEND
213    TAU(I)=TAUS(I)
214    CONTINUE
      NTM=NTIME(IT)*THALF

```

```

C      CALL TRANS (IS2,IDH,IEND,DT)
      DO 27 NT=1,NTM
        CALL DAKT (TIME,IDH,IEND)
        CALL CHEMIE (IDH,IEND,ITYP)
        CALL EULER (DT,IDH,IEND,IS2)
        IF (ID.EQ.1) GOTO 201
        TIME=TIME+DT/3600.
        IF (TIME.GT.24.1) TIME=TIME-24.
        DO 21 I=IANF,IEND,IDH
          LTIME(I)=LTIME(I)+DT/3600.*TAU(I)
          IF (LTIME(I).GT.24.1) LTIME(I)=LTIME(I)-24.
21      CONTINUE

C      CALCULATION OF CONCENTRATIONS OF GROUP MEMBERS
C      -----
C
201     CONTINUE
        DO 205 J=2,8
          KE=NSUM(J-1)
          DO 203 I=IANF,IEND,IDH
203         XALT(I,J)=0.
          DO 205 K=1,KE
            KX=NFAM(K,J-1)
            DO 205 I=IANF,IEND,IDH
              XALT(I,J)=XALT(I,J)+C2(I,KX)
205         CONTINUE
          DO 25 J=2,8
            KE=NSUM(J-1)
            DO 25 K=1,KE
              KX=NFAM(K,J-1)
              DO 25 I=IANF,IEND,IDH
                C2(I,KX)=C2(I,KX)*C1(I,J)/XALT(I,J)
25         CONTINUE
          IX=IMX*(ID/NTAG)+1
          GOTO (259,251),IX
251        IF (TIME.LT.TIMV) GOTO 259
          IF (IMIN.GT.1)
            *      CALL OUTMIN (IMIN,LTIME,IS1,IDH,IEND)
          TIMV=TIME+1./60.
          IF (TIMV.GT.24.) TIMV=1./60.
259        CONTINUE
          IF ((TIME.LT.TVM).OR.(ID.NE.NTAG)) GOTO 27
          IF (IMEAN.EQ.1) CALL MEAN (IDH,IS1)
          TVM=TVM+1.
          IF (TVM.GT.24.) TVM=0.999999

27      CONTINUE
        CALL OUTDIU (IT,IDH,IEND,IS1)
        IF (ID.EQ.NTAG) CALL OUTPT (TIME,IS2,IDH,IEND,ITYP)

C      INTERMEDIATE OUTPUT
C      -----
C
      IF ((ID.EQ.NTAG).AND.(ABS(TIME-12.).LT.0.0000001)) THEN
        IS=90
        WRITE(11) IS
        WRITE(11) C1
        WRITE(11) C2
      ENDIF
      IF ((INTOUT*ID).LT.2) GOTO 28
      IF (ABS(TIME-TV).GT.0.000002) GOTO 28

C
      IS=91
      WRITE(11) IS

```

```
        WRITE(11) TIME
        WRITE(11) C1
        WRITE(11) C2
C
28      CONTINUE
        ITS=1
        IT=20
        IF (ID.EQ.(NTAG-1)) CALL OUTDIU (IT,IDH,IEND,IS3)
29      CONTINUE
C
        IS=9
        WRITE(11) IS
        WRITE(11) IT
        WRITE(11) C1
        WRITE(11) C2
        CALL OUTDIU (IT,IDH,IEND,IS2)
C
        CALL OUTPT (TIME,IS1,IDH,IEND,ITYP)
        TIME=12.
        CALL DAKT (TIME,IDH,IEND)
        IF (IMEAN.EQ.1) CALL MEAN (IDH,IS2)
        IF (IMIN.GT.1) CALL OUTMIN (IMIN,LTIME,IS2,IDH,IEND)
C
C      FORMATE
C      -----
C
2000     FORMAT (10I5)
2020     FORMAT (I5,1P,10E12.2)
2021     FORMAT (I5,1P,E12.2)
2022     FORMAT (1P,10E12.2)
2030     FORMAT ('1')
2040     FORMAT (14I9/OP,14F9.4/1P,14E9.2/)
        RETURN
        END
/*
```

```
//ICH301D4 JOB (324,035431),ROETH,CLASS=C,TIME=(00,19)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D4,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1536K
//C.SYSIN DD *
```

```
C
C
C          DDD      4  4
C          D  D     4  4
C          D  D     44444
C          DDD      4
```

```
C *****
C *
C *      UNTERPROGRAMM: PRODUCTION AND DESTRUCTION RATES *
C *
C *****
```

```
C
C PURPOSE          : CALCULATION OF THE PRODUCTION RATES AND
C                   DESTRUCTION FREQUENCIES FOR GASPHASE AND
C                   WET CHEMISTRY REACTIONS
C INPUT VIA CALL   : IDH: ALTITUDINAL STEP
C                   ITYP: TYPE OF VERSION (STEADY STATE =1;
C                   LONGTERM =2; DIURNAL VARIATION=3)
C INPUT VIA COMMON : PLIGHT: NOX PRODUCTION BY LIGHTNING
C                   PSST: NOX PRODUCTION BY SUBSONIC AIRCRAFTS
C                   PVULK: SO2-PRODUCTION BY VOLCANOES
C                   TEMP: TEMPERATURE
C                   DZ: ALTITUDINAL SPACING
C                   R: ACTUAL GASPHASE REACTION COEFFICIENTS
C                   RN: COEFFICIENTS OF WET CHEMISTRY REACTIONS
C                   C: CONCENTRATIONS OF THE AIR'S COMPOUNDS
C                   ICHECK: SWITCH  =0: NO CHECK
C                               =1: CHECK FOR H AND CL ATOMS
C OUTPUT VIA COMMON: PC: INDIVIDUAL PRODUCTION RATES
C                   DC: INDIVIDUAL DESTRUCTION FREQUENCIES
```

```
      SUBROUTINE CHEMIE (IDH,IEND,ITYP)
```

```
C
C
C      IMPLICIT REAL*8 (A-H,O-Z)
```

```
      COMMON-BEREICHE
```

```
      -----
      COMMON /RAIN/   PHW,PVULK(0:99),PLIGHT(0:99),PSST(0:99),PRB(0:99)
      COMMON /MET/    EDD(0:99),TEMP(0:99),DZ
      COMMON /RATEAK/  R(200,0:99),D(70,0:99),RN(20,0:99)
      COMMON /CONC/    C1(0:99,0:33),C2(0:99,1:30)
      COMMON /TERME/   PC1(0:99,2:33), PC2(0:99,1:30),
*                    DC1(0:99,2:33), DC2(0:99,1:30), TT(0:99,2:33)
      COMMON /ISWTCH/  IP(12)
```

```
      EQUIVALENCE
```

```
      -----
      EQUIVALENCE      (AM (0), C1(0, 0)),( O2 (0), C1(0, 1)),
1( ODD (0), C1(0, 2)),(ANODD (0), C1(0, 3)),( HODD (0), C1(0, 4)),
2( SOX (0), C1(0, 5)),( HXS (0), C1(0, 6)),( CLX (0), C1(0, 7)),
3( CW (0), C1(0, 8)),( DUM1 (0), C1(0, 9)),( DUM2 (0), C1(0,10)),
4(AN2O (0), C1(0,11)),(ANH3 (0), C1(0,12)),(ANH4 (0), C1(0,13)),
5( HNO3 (0), C1(0,14)),( H2 (0), C1(0,15)),( H2O (0), C1(0,16)),
6( WSSR (0), C1(0,17)),( H2O2 (0), C1(0,18)),( H2SO4(0), C1(0,19)),
7( COS (0), C1(0,20)),( CO (0), C1(0,21)),( CO2 (0), C1(0,22)),
```

8(CH4 (0), C1(0,23)), (C2H2 (0), C1(0,24)), (C2H6 (0), C1(0,25)),
 9(C3H8 (0), C1(0,26)), (F11 (0), C1(0,27)), (F12 (0), C1(0,28)),
 A(CCL4 (0), C1(0,29)), (CH3CL(0), C1(0,30)), (CHCL3(0), C1(0,31)),
 B(C2CL3(0), C1(0,32)), (HCL (0), C1(0,33))

C
 EQUIVALENCE (O (0), C2(0, 1)),
 1(OS (0), C2(0, 2)), (O3 (0), C2(0, 3)), (AN (0), C2(0, 4)),
 2(ANO (0), C2(0, 5)), (ANO2 (0), C2(0, 6)), (ANO3 (0), C2(0, 7)),
 3(AN2O5 (0), C2(0, 8)), (HNO2 (0), C2(0, 9)), (HNO4 (0), C2(0,10)),
 4(H (0), C2(0,11)), (OH (0), C2(0,12)), (HO2 (0), C2(0,13)),
 5(SO (0), C2(0,14)), (SO2 (0), C2(0,15)), (HS (0), C2(0,16)),
 6(H2S (0), C2(0,17)), (CL (0), C2(0,18)), (CLO (0), C2(0,19)),
 7(CL2 (0), C2(0,20)), (HOCL (0), C2(0,21)), (CLNO3(0), C2(0,22)),
 8(CHO (0), C2(0,23)), (CH3 (0), C2(0,24)), (CH2O (0), C2(0,25)),
 9(CH3O (0), C2(0,26)), (CH3O2(0), C2(0,27)), (DUM3 (0), C2(0,28)),
 A(DUM4 (0), C2(0,29)), (DUM5 (0), C2(0,30))

C
 EQUIVALENCE
 1(PODD (0),PC1(0, 2)), (PNODD (0),PC1(0, 3)), (PHODD (0),PC1(0, 4)),
 2(PSOX (0),PC1(0, 5)), (PHXS (0),PC1(0, 6)), (PCLX (0),PC1(0, 7)),
 3(PCW (0),PC1(0, 8)), (PDUM1 (0),PC1(0, 9)), (PDUM2 (0),PC1(0,10)),
 4(PN2O (0),PC1(0,11)), (PNH3 (0),PC1(0,12)), (PNH4 (0),PC1(0,13)),
 5(PHNO3 (0),PC1(0,14)), (PH2 (0),PC1(0,15)), (PH2O (0),PC1(0,16)),
 6(PWSSR (0),PC1(0,17)), (PH2O2 (0),PC1(0,18)), (PH2SO4(0),PC1(0,19)),
 7(PCOS (0),PC1(0,20)), (PCO (0),PC1(0,21)), (PCO2 (0),PC1(0,22)),
 8(PCH4 (0),PC1(0,23)), (PC2H2 (0),PC1(0,24)), (PC2H6 (0),PC1(0,25)),
 9(PC3H8 (0),PC1(0,26)), (PF11 (0),PC1(0,27)), (PF12 (0),PC1(0,28)),
 A(PCCL4 (0),PC1(0,29)), (PCH3CL(0),PC1(0,30)), (PCHCL3(0),PC1(0,31)),
 B(PC2CL3(0),PC1(0,32)), (PHCL (0),PC1(0,33))

C
 EQUIVALENCE (PO (0),PC2(0, 1)),
 1(POS (0),PC2(0, 2)), (PO3 (0),PC2(0, 3)), (PN (0),PC2(0, 4)),
 2(PNO (0),PC2(0, 5)), (PNO2 (0),PC2(0, 6)), (PNO3 (0),PC2(0, 7)),
 3(PN2O5 (0),PC2(0, 8)), (PHNO2 (0),PC2(0, 9)), (PHNO4 (0),PC2(0,10)),
 4(PH (0),PC2(0,11)), (POH (0),PC2(0,12)), (PHO2 (0),PC2(0,13)),
 5(PSO (0),PC2(0,14)), (PSO2 (0),PC2(0,15)), (PHS (0),PC2(0,16)),
 6(PH2S (0),PC2(0,17)), (PCL (0),PC2(0,18)), (PCLO (0),PC2(0,19)),
 7(PCL2 (0),PC2(0,20)), (PHOCL (0),PC2(0,21)), (PCLNO3(0),PC2(0,22)),
 8(PCHO (0),PC2(0,23)), (PCH3 (0),PC2(0,24)), (PCH2O (0),PC2(0,25)),
 9(PCH3O (0),PC2(0,26)), (PCH3O2(0),PC2(0,27)), (PDUM3 (0),PC2(0,28)),
 A(PDUM4 (0),PC2(0,29)), (PDUM5 (0),PC2(0,30))

C
 EQUIVALENCE
 1(DODD (0),DC1(0, 2)), (DNODD (0),DC1(0, 3)), (DHODD (0),DC1(0, 4)),
 2(DSOX (0),DC1(0, 5)), (DHXS (0),DC1(0, 6)), (DCLX (0),DC1(0, 7)),
 3(DCW (0),DC1(0, 8)), (DDUM1 (0),DC1(0, 9)), (DDUM2 (0),DC1(0,10)),
 4(DN2O (0),DC1(0,11)), (DNH3 (0),DC1(0,12)), (DNH4 (0),DC1(0,13)),
 5(DHNO3 (0),DC1(0,14)), (DH2 (0),DC1(0,15)), (DH2O (0),DC1(0,16)),
 6(DWSSR (0),DC1(0,17)), (DH2O2 (0),DC1(0,18)), (DH2SO4(0),DC1(0,19)),
 7(DCOS (0),DC1(0,20)), (DCO (0),DC1(0,21)), (DCO2 (0),DC1(0,22)),
 8(DCH4 (0),DC1(0,23)), (DC2H2 (0),DC1(0,24)), (DC2H6 (0),DC1(0,25)),
 9(DC3H8 (0),DC1(0,26)), (DF11 (0),DC1(0,27)), (DF12 (0),DC1(0,28)),
 A(DCCL4 (0),DC1(0,29)), (DCH3CL(0),DC1(0,30)), (DCHCL3(0),DC1(0,31)),
 B(DC2CL3(0),DC1(0,32)), (DHCL (0),DC1(0,33))

C
 EQUIVALENCE (DO (0),DC2(0, 1)),
 1(DOS (0),DC2(0, 2)), (DO3 (0),DC2(0, 3)), (DN (0),DC2(0, 4)),
 2(DNO (0),DC2(0, 5)), (DNO2 (0),DC2(0, 6)), (DNO3 (0),DC2(0, 7)),
 3(DN2O5 (0),DC2(0, 8)), (DHNO2 (0),DC2(0, 9)), (DHNO4 (0),DC2(0,10)),
 4(DH (0),DC2(0,11)), (DOH (0),DC2(0,12)), (DHO2 (0),DC2(0,13)),
 5(DSO (0),DC2(0,14)), (DSO2 (0),DC2(0,15)), (DHS (0),DC2(0,16)),
 6(DH2S (0),DC2(0,17)), (DCL (0),DC2(0,18)), (DCLO (0),DC2(0,19)),

7(DCL2 (0),DC2(0,20)),(DHOCL (0),DC2(0,21)),(DCLNO3(0),DC2(0,22)),
 8(DCHO (0),DC2(0,23)),(DCH3 (0),DC2(0,24)),(DCH2O (0),DC2(0,25)),
 9(DCH3O (0),DC2(0,26)),(DCH3O2(0),DC2(0,27)),(DDUM3 (0),DC2(0,28)),
 A(DDUM4 (0),DC2(0,29)),(DDUM5 (0),DC2(0,30))

DIMENSIONEN

REAL *8 AM (0:99), O2 (0:99), ODD (0:99), ANODD (0:99),
 1 HODD (0:99), SOX (0:99), HXS (0:99), CLX (0:99),
 2 CW (0:99), DUM1 (0:99), DUM2 (0:99), AN2O (0:99),
 3 ANH3 (0:99), ANH4 (0:99), HNO3 (0:99), H2 (0:99),
 4 H2O (0:99), WSSR (0:99), H2O2 (0:99), H2SO4(0:99),
 5 COS (0:99), CO (0:99), CO2 (0:99), CH4 (0:99),
 6 C2H2 (0:99), C2H6 (0:99), C3H8 (0:99), F11 (0:99),
 7 F12 (0:99), CCL4 (0:99), CH3CL(0:99), CHCL3(0:99),
 8 C2CL3(0:99), HCL (0:99)

REAL *8 O (0:99), OS (0:99), O3 (0:99), AN (0:99),
 1 ANO (0:99), ANO2 (0:99), ANO3 (0:99), AN2O5 (0:99),
 2 HNO2 (0:99), HNO4 (0:99), H (0:99), OH (0:99),
 3 HO2 (0:99), SO (0:99), SO2 (0:99), HS (0:99),
 4 H2S (0:99), CL (0:99), CLO (0:99), CL2 (0:99),
 5 HOCL (0:99), CLNO3(0:99), CHO (0:99), CH3 (0:99),
 6 CH2O (0:99), CH3O (0:99), CH3O2(0:99), DUM3 (0:99),
 7 DUM4 (0:99), DUM5 (0:99)

REAL *8 PODD (0:99), PNODD (0:99),
 1 PHODD (0:99), PSOX (0:99), PHXS (0:99), PCLX (0:99),
 2 PCW (0:99), PDUM1 (0:99), PDUM2 (0:99), PN2O (0:99),
 3 PNH3 (0:99), PNH4 (0:99), PHNO3 (0:99), PH2 (0:99),
 4 PH2O (0:99), PWSSR (0:99), PH2O2 (0:99), PH2SO4(0:99),
 5 PCOS (0:99), PCO (0:99), PCO2 (0:99), PCH4 (0:99),
 6 PC2H2 (0:99), PC2H6 (0:99), PC3H8 (0:99), PF11 (0:99),
 7 PF12 (0:99), PCCL4 (0:99), PCH3CL(0:99), PCHCL3(0:99),
 8 PC2CL3(0:99), PHCL (0:99)

REAL *8 PO (0:99), POS (0:99), PO3 (0:99), PN (0:99),
 1 PNO (0:99), PNO2 (0:99), PNO3 (0:99), PN2O5 (0:99),
 2 PHNO2 (0:99), PHNO4 (0:99), PH (0:99), POH (0:99),
 3 PHO2 (0:99), PSO (0:99), PSO2 (0:99), PHS (0:99),
 4 PH2S (0:99), PCL (0:99), PCLO (0:99), PCL2 (0:99),
 5 PHOCL (0:99), PCLNO3(0:99), PCHO (0:99), PCH3 (0:99),
 6 PCH2O (0:99), PCH3O (0:99), PCH3O2(0:99), PDUM3 (0:99),
 7 PDUM4 (0:99), PDUM5 (0:99)

REAL *8 DODD (0:99), DNODD (0:99),
 1 DHODD (0:99), DSOX (0:99), DHXS (0:99), DCLX (0:99),
 2 DCW (0:99), DDUM1 (0:99), DDUM2 (0:99), DN2O (0:99),
 3 DNH3 (0:99), DNH4 (0:99), DHNO3 (0:99), DH2 (0:99),
 4 DH2O (0:99), DWSSR (0:99), DH2O2 (0:99), DH2SO4(0:99),
 5 DCOS (0:99), DCO (0:99), DCO2 (0:99), DCH4 (0:99),
 6 DC2H2 (0:99), DC2H6 (0:99), DC3H8 (0:99), DF11 (0:99),
 7 DF12 (0:99), DCCL4 (0:99), DCH3CL(0:99), DCHCL3(0:99),
 8 DC2CL3(0:99), DHCL (0:99)

REAL *8 DO (0:99), DOS (0:99), DO3 (0:99), DN (0:99),
 1 DNO (0:99), DNO2 (0:99), DNO3 (0:99), DN2O5 (0:99),
 2 DHNO2 (0:99), DHNO4 (0:99), DH (0:99), DOH (0:99),
 3 DHO2 (0:99), DSO (0:99), DSO2 (0:99), DHS (0:99),
 4 DH2S (0:99), DCL (0:99), DCLO (0:99), DCL2 (0:99),
 5 DHOCL (0:99), DCLNO3(0:99), DCHO (0:99), DCH3 (0:99),
 6 DCH2O (0:99), DCH3O (0:99), DCH3O2(0:99), DDUM3 (0:99),
 7 DDUM4 (0:99), DDUM5 (0:99)

1 FORMAT (3I5,1P,8E14.5)

2 FORMAT (1P,10E12.2)

DATA NIX/0/

CALL MASKE

IANF=0

JE=3

IF (ITYP.EQ.3) JE=1

PRODUCTION- AND DESTRUCTIONRATES WITIN THE FAMILIES

DO 99 JJ=1,JE

SAUERSTOFF

DO 19 I=IANF,IEND,IDH

PO(I)=R(31,I)*O2(I)*SO(I)+R(29,I)*O2(I)*AN(I)

1 +R(44,I)*AN(I)*ANO(I)+R(65,I)*OH(I)*OH(I)

2 +D(4,I)*ANO(I)+D(5,I)*ANO2(I)+D(6,I)*ANO3(I)+D(9,I)*AN2O5(I)

3 +2.*D(1,I)*O2(I)+D(15,I)*SO2(I)+D(26,I)*HO2(I)+D(16,I)*CLO(I)

4 +D(18,I)*CO2(I)+D(28,I)*HOCL(I)+D(30,I)*CH3O2(I)

5 +R(193,I)*CL(I)*CLNO3(I)+R(45,I)*AN(I)*ANO2(I)

PODD(I)=PO(I)

PO(I)=PO(I)+R(18,I)*OS(I)*O2(I)+R(19,I)*OS(I)*(AM(I)-O2(I))

1 +R(194,I)*OS(I)*CO2(I)+2.*R(196,I)*OS(I)*O3(I)+D(3,I)*O3(I)

DO(I)=R(2,I)*O3(I)+R(3,I)*ANO(I)+R(4,I)*ANO2(I)+R(5,I)*ANO2(I)

1 +R(6,I)*ANO3(I)+R(8,I)*OH(I)+R(9,I)*HO2(I)+R(198,I)*HNO4(I)

2 +R(10,I)*H2O2(I)+R(11,I)*SO2(I)+R(12,I)*CLO(I)+R(13,I)*CH2O(I)

3 +R(14,I)*CH3(I)+R(16,I)*CH3CL(I)+R(17,I)*CLNO3(I)

4 +R(89,I)*HOCL(I)+R(62,I)*COS(I)+R(96,I)*H2S(I)+R(172,I)*C2H2(I)

5 +R(199,I)*H2O(I)+R(124,I)*HS(I)

6 +2.*R(101,I)*O(I)+R(102,I)*AN(I)+R(103,I)*H2(I)

7 +R(105,I)*SO(I)+R(106,I)*HCL(I)+R(107,I)*CHO(I)+R(108,I)*CH4(I)

DODD(I)=DO(I)*O(I)

DO(I)=DO(I)+R(1,I)*O2(I)

POS(I)=D(8,I)*AN2O(I)

PODD(I)=PODD(I)+POS(I)

POS(I)=POS(I)+D(2,I)*O3(I)

DOS(I)=R(21,I)*AN2O(I)+R(22,I)*AN2O(I)+R(28,I)*F11(I)

1+R(26,2)*CH4(I)+R(24,I)*H2O(I)+R(23,I)*H2(I)+R(20,I)*(AM(I)-O2(I))

2 +R(27,I)*F12(I)+R(94,I)*COS(I)+R(195,I)*ANH3(I)+R(189,I)*CCL4(I)

3 +R(179,I)*C3H8(I)+R(182,I)*C2H2(I)+R(185,I)*C2H6(I)

4 +R(197,I)*O3(I)+R(25,I)*CH4(I)

5 +R(110,I)*HCL(I)+R(109,I)*H2O2(I)

DODD(I)=DODD(I)+DOS(I)*OS(I)

DOS(I)=DOS(I)+R(18,I)*O2(I)+R(19,I)*(AM(I)-O2(I))+R(194,I)*CO2(I)

1 +R(196,I)*O3(I)

PO3(I)=0.

PODD(I)=PODD(I)+PO3(I)

PO3(I)=PO3(I)+R(1,I)*O2(I)*O(I)

DO3(I)=R(2,I)*O(I)+R(43,I)*CL(I)+R(42,I)*SO(I)+R(41,I)*HO2(I)

1 +R(40,I)*OH(I)+R(39,I)*H(I)+R(37,I)*ANO(I)+R(36,I)*AN(I)

2 +R(38,I)*ANO2(I)+R(97,I)*HS(I)+R(171,I)*CH3(I)+R(197,I)*OS(I)

DODD(I)=DODD(I)+DO3(I)*O3(I)

DO3(I)=DO3(I)+D(2,I)+D(3,I)+R(196,I)*OS(I)

DODD(I)=DODD(I)/ODD(I)

19 CONTINUE

STICKSTOFF

DO 29 I=IANF,IEND,IDH

PN(I)=0.

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PNODD(I)=PN(I)
PN(I)=PN(I)+D(4,I)*ANO(I)
DN(I)=R(45,I)*ANO2(I)+R(44,I)*ANO(I)
DNODD(I)=DN(I)*AN(I)
DN(I)=DN(I)+R(29,I)*O2(I)+R(36,I)*O3(I)
1 +R(111,I)*OH(I)+R(102,I)*O(I)
PNO(I)=2.*R(22,I)*OS(I)*AN2O(I)
PNODD(I)=PNODD(I)+PNO(I)
PNO(I)=PNO(I)+R(4,I)*O(I)*ANO2(I)+R(29,I)*O2(I)*AN(I)
1 +D(5,I)*ANO2(I)+D(7,I)*ANO3(I)+D(32,I)*HNO2(I)
2 +R(111,I)*AN(I)*OH(I)+R(113,I)*ANO2(I)*H(I)+R(102,I)*O(I)*AN(I)
3 +R(36,I)*O3(I)*AN(I)
DNO(I)=R(49,I)*HO2(I)+R(44,I)*AN(I)
DNODD(I)=DNODD(I)+DNO(I)*ANO(I)
DNO(I)=DNO(I)+R(3,I)*O(I)+R(37,I)*O3(I)+R(51,I)*CH3O2(I)
1 +R(48,I)*HO2(I)+R(46,I)*ANO3(I)+D(4,I)+R(47,I)*OH(I)
2 +R(50,I)*CLO(I)
PNO2(I)=D(14,I)*HNO3(I)+D(10,I)*ANH3(I)+R(61,I)*ANH3(I)*OH(I)
1 +R(195,I)*OS(I)*ANH3(I)
PNODD(I)=PNODD(I)+PNO2(I)
PNO2(I)=PNO2(I)+R(3,I)*O(I)*ANO(I)+R(6,I)*O(I)*ANO3(I)
1 +R(37,I)*O3(I)*ANO(I)+R(51,I)*ANO(I)*CH3O2(I)
2 +R(48,I)*ANO(I)*HO2(I)+2.*R(46,I)*ANO(I)*ANO3(I)
3 +D(6,I)*ANO3(I)+R(50,I)*ANO(I)*CLO(I)
4 +R(15,I)*OH(I)*HNO4(I)+R(52,I)*CL(I)*HNO4(I)
5 +R(57,I)*(AM(I)*.21)*HNO4(I)+R(59,I)*AN2O5(I)
6 +R(69,I)*OH(I)*HNO2(I)+R(193,I)*CL(I)*CLNO3(I)
7 +R(198,I)*O(I)*HNO4(I)+2.*D(9,I)*AN2O5(I)
8 +D(31,I)*HNO2(I)+D(33,I)*HNO4(I)
DNO2(I)=R(45,I)*AN(I)+R(53,I)*OH(I)
DNODD(I)=DNODD(I)+DNO2(I)*ANO2(I)
DNO2(I)=DNO2(I)+R(4,I)*O(I)+R(5,I)*O(I)+R(38,I)*O3(I)+D(5,I)
1 +R(113,I)*H(I)+R(7,I)*HO2(I)+R(54,I)*HO2(I)+R(55,I)*ANO3(I)
2 +R(56,I)*CLO(I)+R(114,I)*CH3O(I)
PNO3(I)=R(70,I)*HNO3(I)*OH(I)+R(112,I)*HNO3(I)*CL(I)
PNODD(I)=PNODD(I)+PNO3(I)
PNO3(I)=PNO3(I)+R(5,I)*O(I)*ANO2(I)+R(38,I)*O3(I)*ANO2(I)
1 +R(17,I)*CLNO3(I)*O(I)+R(59,I)*AN2O5(I)
2 +D(25,I)*CLNO3(I)
DNO3(I)=0.
DNODD(I)=DNODD(I)+DNO3(I)*ANO3(I)
DNO3(I)=DNO3(I)+R(6,I)*O(I)+R(46,I)*ANO(I)+D(6,I)+D(7,I)
1 +R(55,I)*ANO2(I)
PN2O5(I)=0.
PNODD(I)=PNODD(I)+2.*PN2O5(I)
PN2O5(I)=PN2O5(I)+R(55,I)*ANO2(I)*ANO3(I)
DN2O5(I)=R(60,I)*H2O(I)
DNODD(I)=DNODD(I)+2.*DN2O5(I)*AN2O5(I)
DN2O5(I)=DN2O5(I)+R(59,I)+D(9,I)
PHNO2(I)=0.
PNODD(I)=PNODD(I)+PHNO2(I)
PHNO2(I)=PHNO2(I)+R(47,I)*ANO(I)*OH(I)+R(54,I)*ANO2(I)*HO2(I)
1 +R(114,I)*ANO2(I)*CH3O(I)
DHNO2(I)=0.
DNODD(I)=DNODD(I)+DHNO2(I)*HNO2(I)
DHNO2(I)=DHNO2(I)+R(69,I)*OH(I)+D(31,I)+D(32,I)
PHNO4(I)=0.
PNODD(I)=PNODD(I)+PHNO4(I)
PHNO4(I)=PHNO4(I)+R(7,I)*ANO2(I)*HO2(I)
DHNO4(I)=0.
DNODD(I)=DNODD(I)+DHNO4(I)*HNO4(I)
DHNO4(I)=DHNO4(I)+R(15,I)*OH(I)+R(52,I)*CL(I)+R(57,I)*(AM(I)*.21)
1 +R(198,I)*O(I)+D(33,I)

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C      CLNO3:
      PNODD(I)=PNODD(I)+0.
      DNODD(I)=DNODD(I)+R(81,I)*OH(I)*CLNO3(I)
      DNODD(I)=DNODD(I)/ANODD(I)
29 CONTINUE

C
C      WASSERSTOFF
C      -----
      DO 39 I=IANF,IEND,IDH
      PH(I)=R(14,I)*O(I)*CH3(I)+R(23,I)*OS(I)*H2(I)
1      +D(10,I)*ANH3(I)+D(11,I)*H2O(I)+D(20,I)*CH2O(I)+D(17,I)*HCL(I)
2      +R(85,I)*H2(I)*CL(I)+R(124,I)*O(I)*HS(I)
3      +R(103,I)*O(I)*H2(I)
      PHODD(I)=PH(I)
      PH(I)=PH(I)+R(8,I)*O(I)*OH(I)+R(73,I)*OH(I)*CO(I)
1      +R(67,I)*OH(I)*H2(I)+D(31,I)*HNO2(I)+R(74,I)*OH(I)*CO(I)
2      +R(111,I)*AN(I)*OH(I)
      DH(I)=R(63,I)*HO2(I)+R(64,I)*HO2(I)
1      +R(118,I)*HCL(I)+2.*R(115,I)*H(I)
      DHODD(I)=DH(I)*H(I)
      DH(I)=DH(I)+R(30,I)*O2(I)+R(39,I)*O3(I)
1      +R(113,I)*ANO2(I)+R(116,I)*H2O2(I)+R(117,I)*H2O2(I)
      POH(I)=R(10,I)*O(I)*H2O2(I)+R(13,I)*O(I)*CH2O(I)
1+R(26,I)*OS(I)*CH4(I)+2.*R(24,I)*OS(I)*H2O(I)+R(23,I)*OS(I)*H2(I)
2      +R(34,I)*O2(I)*CH3(I)+2.*D(12,I)*H2O2(I)
3      +D(14,I)*HNO3(I)+D(11,I)*H2O(I)
4      +R(96,I)*H2S(I)*O(I)
5      +R(171,I)*O3(I)*CH3(I)+R(195,I)*OS(I)*ANH3(I)
6      +2.*R(199,I)*O(I)*H2O(I)
7      +R(106,I)*O(I)*HCL(I)+R(107,I)*O(I)*CHO(I)+R(110,I)*OS(I)*HCL(I)
8      +R(108,I)*O(I)*CH4(I)+R(109,I)*OS(I)*H2O2(I)+R(103,I)*O(I)*H2(I)
9      +2.5D-18*O3(I)*DUM1(I)
      PHODD(I)=PHODD(I)+POH(I)
      POH(I)=POH(I)+R(9,I)*O(I)*HO2(I)+R(41,I)*O3(I)*HO2(I)
1      +R(48,I)*ANO(I)*HO2(I)+R(83,I)*HO2(I)*SO2(I)+R(39,I)*O3(I)*H(I)
2      +R(173,I)*HO2(I)*CL(I)+R(192,I)*HO2(I)*CH3O2(I)
3      +R(113,I)*ANO2(I)*H(I)+R(117,I)*H(I)*H2O2(I)+D(26,I)*HO2(I)
4      +R(89,I)*O(I)*HOCL(I)+R(198,I)*O(I)*HNO4(I)
5      +D(27,I)*HOCL(I)+D(32,I)*HNO2(I)+2.*R(64,I)*H(I)*HO2(I)
      DOH(I)=R(61,I)*ANH3(I)+R(79,I)*CCL4(I)+R(77,I)*F12(I)
1      +R(80,I)*CH3CL(I)+R(75,I)*CH2O(I)+R(76,I)*CH4(I)+R(176,I)*HO2(I)
2      +R(81,I)*CLNO3(I)+R(72,I)*HCL(I)+R(70,I)*HNO3(I)+R(69,I)*HNO2(I)
3      +R(66,I)*HO2(I)+2.*R(65,I)*OH(I)+R(71,I)*SO2(I)+R(53,I)*ANO2(I)
4      +R(90,I)*HOCL(I)+R(15,I)*HNO4(I)+R(58,I)*COS(I)
5      +R(95,I)*H2S(I)+R(187,I)*C2H6(I)+R(184,I)*C2H2(I)+R(78,I)*F11(I)
6      +R(181,I)*C3H8(I)+R(178,I)*C2CL3(I)+R(177,I)*CHCL3(I)
7      +2.*R(119,I)*OH(I)
      DHODD(I)=DHODD(I)+DOH(I)*OH(I)
      DOH(I)=DOH(I)+R(8,I)*O(I)+R(40,I)*O3(I)+R(73,I)*CO(I)
1      +R(74,I)*CO(I)+R(68,I)*H2O2(I)+R(67,I)*H2(I)
2      +R(111,I)*AN(I)+R(47,I)*ANO(I)+R(188,I)*CLO(I)
      PHO2(I)=R(10,I)*O(I)*H2O2(I)+R(32,I)*O2(I)*CHO(I)
1      +R(35,I)*O2(I)*CH3O(I)+R(100,I)*HS(I)*H2O2(I)
2      +R(109,I)*OS(I)*H2O2(I)+R(121,I)*H2O2(I)*CL(I)
      PHODD(I)=PHODD(I)+PHO2(I)
      PHO2(I)=PHO2(I)+R(30,I)*O2(I)*H(I)+R(40,I)*O3(I)*OH(I)
1      +R(68,I)*OH(I)*H2O2(I)+R(188,I)*OH(I)*CLO(I)
2      +R(116,I)*H(I)*H2O2(I)+R(57,I)*(AM(I)*.21)*HNO4(I)
3      +D(33,I)*HNO4(I)
      DHO2(I)=R(49,I)*ANO(I)+R(63,I)*H(I)
1      +R(64,I)*H(I)+R(66,I)*OH(I)+R(84,I)*CL(I)+2.*R(82,I)*HO2(I)
2      +R(92,I)*CH2O(I)+R(98,I)*HS(I)+R(99,I)*HS(I)
3      +R(176,I)*OH(I)+2.*R(175,I)*HO2(I)

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DHODD(I)=DHODD(I)+DHO2(I)*HO2(I)
DHO2(I)=DHO2(I)+R(9,I)*O(I)+R(41,I)*O3(I)+R(48,I)*ANO(I)
1      +D(26,I)+R(173,I)*CL(I)+R(192,I)*CH3O2(I)+R(7,I)*ANO2(I)
2      +R(91,I)*CLO(I)+R(54,I)*ANO2(I)+R(83,I)*SO2(I)
C      HNO2:
PHODD(I)=PHODD(I)+R(114,I)*ANO2(I)*CH3O(I)
DHODD(I)=DHODD(I)+R(69,I)*OH(I)*HNO2(I)
C      HNO4:
PHODD(I)=PHODD(I)+0.
DHODD(I)=DHODD(I)+R(15,I)*OH(I)*HNO4(I)+R(52,I)*CL(I)*HNO4(I)
C      HOCL:
PHODD(I)=PHODD(I)+0.
DHODD(I)=DHODD(I)+R(90,I)*OH(I)*HOCL(I)+R(174,I)*CL(I)*HOCL(I)
1      +D(28,I)*HOCL(I)
DHODD(I)=DHODD(I)/HODD(I)
39 CONTINUE
C
C      SCHWEFEL
C      -----
DO 49 I=IANF,IEND,IDH
PSO(I)=R(98,I)*HS(I)*HO2(I)+R(62,I)*O(I)*COS(I)
1      +R(124,I)*O(I)*HS(I)
PSOX(I)=PSO(I)
PSO(I)=PSO(I)+D(15,I)*SO2(I)
DSO(I)=0.
DSOX(I)=DSO(I)*SO(I)
DSO(I)=DSO(I)+R(31,I)*O2(I)+R(42,I)*O3(I)
1      +R(105,I)*O(I)
PSO2(I)=D(13,I)*COS(I)+R(94,I)*COS(I)*OS(I)
1      +R(97,I)*HS(I)*O3(I)+PVULK(I)
PSOX(I)=PSOX(I)+PSO2(I)
PSO2(I)=PSO2(I)+R(31,I)*O2(I)*SO(I)+R(42,I)*O3(I)*SO(I)
1      +R(105,I)*O(I)*SO(I)
DSO2(I)=R(71,I)*OH(I)+R(83,I)*HO2(I)+R(11,I)*O(I)+RN(6,I)
1      +R(120,I)*CH3O2(I)
DSOX(I)=DSOX(I)+DSO2(I)*SO2(I)
DSO2(I)=DSO2(I)+D(15,I)
DSOX(I)=DSOX(I)/SOX(I)
PHS(I)=R(58,I)*COS(I)*OH(I)
PHXS(I)=PHS(I)
PHS(I)=PHS(I)+R(95,I)*H2S(I)*OH(I)+R(96,I)*H2S(I)*O(I)
DHS(I)=R(97,I)*O3(I)+R(98,I)*HO2(I)+R(124,I)*O(I)
DHXS(I)=DHS(I)*HS(I)
DHS(I)=DHS(I)+R(99,I)*HO2(I)+R(100,I)*H2O2(I)
PH2S(I)=0.
PHXS(I)=PHXS(I)+PH2S(I)
PH2S(I)=PH2S(I)+R(99,I)*HS(I)*HO2(I)+R(100,I)*HS(I)*H2O2(I)
DH2S(I)=RN(8,I)
DHXS(I)=DHXS(I)+DH2S(I)*H2S(I)
DH2S(I)=DH2S(I)+R(95,I)*OH(I)+R(96,I)*O(I)
DHXS(I)=DHXS(I)/HXS(I)
49 CONTINUE
C
C      CHLOR
C      -----
DO 69 I=IANF,IEND,IDH
PCL(I)=2.*D(21,I)*F12(I)+3.*D(22,I)*F11(I)+4.*D(23,I)*CCL4(I)
1      +D(24,I)*CH3CL(I)+R(72,I)*OH(I)*HCL(I)+D(17,I)*HCL(I)
2      +R(80,I)*OH(I)*CH3CL(I)
3      +3.*R(177,I)*OH(I)*CHCL3(I)
4      +R(106,I)*O(I)*HCL(I)+R(118,I)*H(I)*HCL(I)+R(110,I)*OS(I)*HCL(I)
PCLX(I)=PCL(I)
PCL(I)=PCL(I)+R(12,I)*O(I)*CLO(I)+R(50,I)*ANO(I)*CLO(I)

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1      +D(16,I)*CLO(I)+R(188,I)*OH(I)*CLO(I)+D(25,I)*CLNO3(I)
2      +D(27,I)*HOCL(I)+2.*D(29,I)*CL2(I)
DCL(I)=R(93,I)*CH2O(I)+R(87,I)*CH4(I)+R(85,I)*H2(I)
1      +R(52,I)*HNO4(I)+R(191,I)*CH3CL(I)+R(186,I)*C2H6(I)
2      +R(183,I)*C2H2(I)+R(180,I)*C3H8(I)
3      +R(84,I)*HO2(I)
4      +R(121,I)*H2O2(I)+R(112,I)*HNO3(I)
DCLX(I)=DCL(I)*CL(I)
DCL(I)=DCL(I)+R(43,I)*O3(I)+R(174,I)*HOCL(I)+R(173,I)*HO2(I)
1      +2.*R(122,I)*CL(I)+R(193,I)*CLNO3(I)
PCLO(I)=R(16,I)*O(I)*CH3CL(I)+2.*R(27,I)*OS(I)*F12(I)
1      +3.*R(28,I)*OS(I)*F11(I)+3.*R(79,I)*OH(I)*CCL4(I)
2      +2.*R(77,I)*OH(I)*F12(I)+3.*R(78,I)*OH(I)*F11(I)
3      +4.*R(189,I)*OS(I)*CCL4(I)+3.*R(178,I)*C2CL3(I)*OH(I)
4      +3.*D(35,I)*C2CL3(I)
PCLX(I)=PCLX(I)+PCLO(I)
PCLO(I)=PCLO(I)+R(43,I)*O3(I)*CL(I)+R(174,I)*CL(I)*HOCL(I)
1      +R(173,I)*CL(I)*HO2(I)+R(17,I)*O(I)*CLNO3(I)
2      +R(89,I)*O(I)*HOCL(I)+R(90,I)*OH(I)*HOCL(I)
3      +R(81,I)*OH(I)*CLNO3(I)
DCLO(I)=0.
DCLX(I)=DCLX(I)+DCLO(I)*CLO(I)
DCLO(I)=DCLO(I)+R(12,I)*O(I)+R(50,I)*ANO(I)+D(16,I)+R(188,I)*OH(I)
1      +R(56,I)*ANO2(I)+R(91,I)*HO2(I)+2.*R(123,I)*CLO(I)
PHOCL(I)=0.
PCLX(I)=PCLX(I)+PHOCL(I)
PHOCL(I)=PHOCL(I)+R(91,I)*HO2(I)*CLO(I)
DHOCL(I)=R(174,I)*CL(I)+D(28,I)
DCLX(I)=DCLX(I)+DHOCL(I)*HOCL(I)
DHOCL(I)=DHOCL(I)+R(89,I)*O(I)+R(90,I)*OH(I)+D(27,I)
PCL2(I)=0.
PCLX(I)=PCLX(I)+2.*PCL2(I)
PCL2(I)=PCL2(I)+R(122,I)*CL(I)*CL(I)+R(123,I)*CLO(I)*CLO(I)
1      +R(193,I)*CL(I)*CLNO3(I)
DCL2(I)=0.
DCLX(I)=DCLX(I)+2.*DCL2(I)*CL2(I)
DCL2(I)=DCL2(I)+D(29,I)
PCLNO3(I)=0.
PCLX(I)=PCLX(I)+PCLNO3(I)
PCLNO3(I)=PCLNO3(I)+R(56,I)*ANO2(I)*CLO(I)
DCLNO3(I)=0.
DCLX(I)=DCLX(I)+DCLNO3(I)*CLNO3(I)
DCLNO3(I)=DCLNO3(I)+R(17,I)*O(I)+R(81,I)*OH(I)+R(193,I)*CL(I)
1      +D(25,I)
DCLX(I)=DCLX(I)/CLX(I)

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KOHLENSTOFF

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PCHO(I)=R(184,I)*OH(I)*C2H2(I)+R(183,I)*CL(I)*C2H2(I)
1      +R(191,I)*CL(I)*CH3CL(I)
2      +2.5D-18*DUM1(I)*O3(I)+D(20,I)*DUM2(I)
PCW(I)=PCHO(I)
PCHO(I)=PCHO(I)+R(13,I)*O(I)*CH2O(I)+R(75,I)*OH(I)*CH2O(I)
1      +R(92,I)*HO2(I)*CH2O(I)+R(93,I)*CL(I)*CH2O(I)+D(20,I)*CH2O(I)
DCHO(I)=R(32,I)*O2(I)
1      +R(107,I)*O(I)
DCW(I)=DCHO(I)*CHO(I)
DCHO(I)=DCHO(I)+0.
PCH2O(I)=R(25,I)*OS(I)*CH4(I)+R(187,I)*C2H6(I)*OH(I)
1      +R(186,I)*C2H6(I)*CL(I)+2.*R(185,I)*C2H6(I)*OS(I)
2      +R(182,I)*C2H2(I)*OS(I)
3      +R(184,I)*C2H2(I)*OH(I)+2.*R(181,I)*C3H8(I)*OH(I)
4      +2.*R(180,I)*C3H8(I)*CL(I)+3.*R(179,I)*C3H8(I)*OS(I)

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5      +R(178,I)*C2CL3(I)*OH(I)+R(172,I)*O(I)*C2H2(I)
PCW(I)=PCW(I)+PCH20(I)
PCH20(I)=PCH20(I)+R(14,I)*O(I)*CH3(I)+R(34,I)*O2(I)*CH3(I)
1      +R(35,I)*O2(I)*CH30(I) +R(171,I)*O3(I)*CH3(I)
2      +R(114,I)*ANO2(I)*CH30(I)
DCH20(I)=D(19,I)+RN(10,I)
DCW(I)=DCW(I)+DCH20(I)*CH20(I)
DCH20(I)=DCH20(I)+R(13,I)*O(I)+R(75,I)*OH(I)+D(20,I)
1      +R(93,I)*CL(I)+R(92,I)*HO2(I)
PCH3(I)=R(16,I)*O(I)*CH3CL(I)+R(26,I)*OS(I)*CH4(I)
1      +R(76,I)*OH(I)*CH4(I)+R(87,I)*CL(I)*CH4(I)
2      +D(24,I)*CH3CL(I)+D(35,I)*C2CL3(I)
3      +R(108,I)*O(I)*CH4(I)
4      +D(20,I)*DUM2(I)
PCW(I)=PCW(I)+PCH3(I)
PCH3(I)=PCH3(I)
1      +R(125,I)*CO(I)*CH30(I)
DCH3(I)=0.
DCW(I)=DCW(I)+DCH3(I)*CH3(I)
DCH3(I)=DCH3(I)+R(14,I)*O(I)+R(33,I)*O2(I)+R(34,I)*O2(I)
1      +R(171,I)*O3(I)
PCH30(I)=R(187,I)*OH(I)*C2H6(I)+R(181,I)*OH(I)*C3H8(I)
1      +R(186,I)*CL(I)*C2H6(I)+R(180,I)*CL(I)*C3H8(I)
PCW(I)=PCW(I)+PCH30(I)
PCH30(I)=PCH30(I)+R(51,I)*ANO(I)*CH302(I)
1      +D(30,I)*CH302(I)+R(192,I)*HO2(I)*CH302(I)
2      +R(120,I)*SO2(I)*CH302(I)+2.*R(88,I)*CH302(I)*CH302(I)
DCH30(I)=0.
DCW(I)=DCW(I)+DCH30(I)*CH30(I)
DCH30(I)=DCH30(I)+R(35,I)*O2(I)
1      +R(125,I)*CO(I)+R(114,I)*ANO2(I)
PCH302(I)=0.
PCW(I)=PCW(I)+PCH302(I)
PCH302(I)=PCH302(I)+R(33,I)*O2(I)*CH3(I)
DCH302(I)=0.
DCW(I)=DCW(I)+DCH302(I)*CH302(I)
DCH302(I)=DCH302(I)+R(51,I)*ANO(I)+2.*R(88,I)*CH302(I)+D(30,I)
1      +R(192,I)*HO2(I)
2      +R(120,I)*SO2(I)
DCW(I)=DCW(I)/CW(I)
69 CONTINUE

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RATIOS WITHIN THE FAMILIES

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IF (JJ.EQ.JE) GOTO 99
RAT=1.-FLOAT(JJ-1)/FLOAT(JE-2)
DO 89 I=IANF,IEND,IDH
O(I)=(PO(I)/DO(I)+O(I)*RAT)/(1.+RAT)
OS(I)=(POS(I)/DOS(I)+OS(I)*RAT)/(1.+RAT)
O3(I)=(PO3(I)/DO3(I)+O3(I)*RAT)/(1.+RAT)
X=ODD(I)/(O(I)+O3(I)+OS(I))
O(I)=O(I)*X
O3(I)=O3(I)*X
OS(I)=OS(I)*X
CL(I)=(PCL(I)/DCL(I)+CL(I)*RAT)/(1.+RAT)
CLO(I)=(PCLO(I)/DCLO(I)+CLO(I)*RAT)/(1.+RAT)
HOCL(I)=(PHOCL(I)/DHOCL(I)+HOCL(I)*RAT)/(1.+RAT)
CLNO3(I)=(PCLNO3(I)/DCLNO3(I)+CLNO3(I)*RAT)/(1.+RAT)
CL2(I)=(PCL2(I)/DCL2(I)+CL2(I)*RAT)/(1.+RAT)
X=CLX(I)/(CL(I)+CLO(I)+HOCL(I)+CLNO3(I)+2.*CL2(I))
XCL=X
CL(I)=CL(I)*X

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CLO(I)=CLO(I)*X
CL2(I)=CL2(I)*X
AN(I)=(PN(I)/DN(I)+AN(I)*RAT)/(1.+RAT)
ANO(I)=(PNO(I)/DNO(I)+ANO(I)*RAT)/(1.+RAT)
ANO2(I)=(PNO2(I)/DNO2(I)+ANO2(I)*RAT)/(1.+RAT)
ANO3(I)=(PNO3(I)/DNO3(I)+ANO3(I)*RAT)/(1.+RAT)
AN2O5(I)=(PN2O5(I)/DN2O5(I)+AN2O5(I)*RAT)/(1.+RAT)
HNO2(I)=(PHNO2(I)/DHNO2(I)+HNO2(I)*RAT)/(1.+RAT)
HNO4(I)=(PHNO4(I)/DHNO4(I)+HNO4(I)*RAT)/(1.+RAT)
X=ANODD(I)/(AN(I)+ANO(I)+ANO2(I)+ANO3(I)
1      +2.*AN2O5(I)+HNO2(I)+HNO4(I)+CLNO3(I))
XN=X
AN(I)=X*AN(I)
ANO(I)=X*ANO(I)
ANO2(I)=X*ANO2(I)
ANO3(I)=X*ANO3(I)
AN2O5(I)=X*AN2O5(I)
H(I)=(PH(I)/DH(I)+H(I)*RAT)/(1.+RAT)
OH(I)=(POH(I)/DOH(I)+OH(I)*RAT)/(1.+RAT)
HO2(I)=(PHO2(I)/DHO2(I)+HO2(I)*RAT)/(1.+RAT)
X=HODD(I)/(HNO2(I)+HNO4(I)+HOCL(I)+H(I)+OH(I)+HO2(I))
XH=X
H(I)=H(I)*X
OH(I)=OH(I)*X
HO2(I)=HO2(I)*X
SO(I)=(PSO(I)/DSO(I)+SO(I)*RAT)/(1.+RAT)
SO2(I)=(PSO2(I)/DSO2(I)+SO2(I)*RAT)/(1.+RAT)
X=SOX(I)/(SO(I)+SO2(I))
SO(I)=SO(I)*X
SO2(I)=SO2(I)*X
HS(I)=(PHS(I)/DHS(I)+HS(I)*RAT)/(1.+RAT)
H2S(I)=(PH2S(I)/DH2S(I)+H2S(I)*RAT)/(1.+RAT)
X=HXS(I)/(HS(I)+H2S(I))
HS(I)=HS(I)*X
H2S(I)=H2S(I)*X
CH3(I)=(PCH3(I)/DCH3(I)+CH3(I)*RAT)/(1.+RAT)
CHO(I)=(PCHO(I)/DCHO(I)+CHO(I)*RAT)/(1.+RAT)
CH2O(I)=(PCH2O(I)/DCH2O(I)+CH2O(I)*RAT)/(1.+RAT)
CH3O(I)=(PCH3O(I)/DCH3O(I)+CH3O(I)*RAT)/(1.+RAT)
CH3O2(I)=(PCH3O2(I)/DCH3O2(I)+CH3O2(I)*RAT)/(1.+RAT)
X=CW(I)/(CH3(I)+CHO(I)+CH3O(I)+CH3O2(I)+CH2O(I))
CH3(I)=CH3(I)*X
CHO(I)=CHO(I)*X
CH2O(I)=CH2O(I)*X
CH3O(I)=CH3O(I)*X
CH3O2(I)=CH3O2(I)*X

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C

TEMPORARY RESERVOIRS

CLNO3(I)=CLNO3(I)*SQRT(XCL*XN)

HOCL(I)=HOCL(I)*SQRT(XCL*XH)

HNO2(I)=HNO2(I)*SQRT(XN*XH)

HNO4(I)=HNO4(I)*SQRT(XN*XH)

89 CONTINUE

99 CONTINUE

C

C

CALCULATION OF PRODUCTION- AND DESTRUCTIONRATES

C

C

SAUERSTOFF

C

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DO 119 I=IANF,IEND,IDH

C

119 CONTINUE

C

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STICKSTOFF

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DO 149 I=IANF,IEND,IDH
PN2O(I)=R(20,I)*OS(I)*(AM(I)-O2(I))+R(45,I)*AN(I)*ANO2(I)
DN2O(I)=R(21,I)*OS(I)+R(22,I)*OS(I)+D(8,I)
PNH3(I)=0.
DNH3(I)=R(61,I)*OH(I)+D(10,I)+R(195,I)*OS(I)+R(190,I)
PNH4(I)=R(190,I)*ANH3(I)
PNH4(I)=0.
DNH4(I)=RN(1,I)
DNH4(I)=0.
ANH4(I)=0.
PHNO3(I)=R(49,I)*ANO(I)*HO2(I)+2.*R(60,I)*AN2O5(I)*H2O(I)
1 +R(81,I)*OH(I)*CLNO3(I)+R(53,I)*ANO2(I)*OH(I)
DHNO3(I)=R(70,I)*OH(I)+D(14,I)+RN(2,I)
1 +R(112,I)*CL(I)
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WASSERSTOFF

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PH2(I)=R(25,I)*OS(I)*CH4(I)+R(63,I)*H(I)*HO2(I)+D(19,I)*CH2O(I)
1 +R(116,I)*H(I)*H2O2(I)+R(115,I)*H(I)*H(I)+R(118,I)*H(I)*HCL(I)
DH2(I)=R(23,I)*OS(I)+R(67,I)*OH(I)+R(85,I)*CL(I)
1 +R(103,I)*O(I)
PH2O(I)=2.*R(61,I)*ANH3(I)*OH(I)
1 +R(76,I)*OH(I)*CH4(I)+R(72,I)*OH(I)*HCL(I)+R(70,I)*OH(I)*HNO3(I)
2 +R(69,I)*OH(I)*HNO2(I)+R(68,I)*OH(I)*H2O2(I)+R(67,I)*OH(I)*H2(I)
3 +R(66,I)*OH(I)*HO2(I)+R(65,I)*OH(I)*OH(I)+R(75,I)*OH(I)*CH2O(I)
4 +R(90,I)*OH(I)*HOCL(I)+2.*R(80,I)*OH(I)*CH3CL(I)
5 +R(15,I)*HNO4(I)*OH(I)+R(95,I)*H2S(I)*OH(I)+R(98,I)*HS(I)*HO2(I)
6 +R(187,I)*C2H6(I)*OH(I)+R(195,I)*ANH3(I)*OS(I)
7 +R(181,I)*C3H8(I)*OH(I)+R(178,I)*C2CL3(I)*OH(I)
8 +R(176,I)*OH(I)*HO2(I)+R(185,I)*OS(I)*C2H6(I)
9 +R(179,I)*OS(I)*C3H8(I)+D(10,I)*ANH3(I)+R(177,I)*OH(I)*CHCL3(I)
A +.5*R(77,I)*OH(I)*F12(I)+.5*R(78,I)*OH(I)*F11(I)
B +R(117,I)*H(I)*H2O2(I)
DH2O(I)=R(24,I)*OS(I)+R(60,I)*AN2O5(I)+D(11,I)+R(199,I)*O(I)
PH2O2(I)=R(82,I)*HO2(I)*HO2(I)+R(92,I)*HO2(I)*CH2O(I)
1 +R(175,I)*HO2(I)*HO2(I)
2 +R(119,I)*OH(I)*OH(I)
DH2O2(I)=R(10,I)*O(I)+R(68,I)*OH(I)+D(12,I)+R(100,I)*HS(I)
1 +R(109,I)*OS(I)+R(116,I)*H(I)+R(117,I)*H(I)+R(121,I)*CL(I)
PWSSR(I)=0.
DWSSR(I)=0.
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SCHWEFEL

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PCOS(I)=0.
DCOS(I)=D(13,I)+R(58,I)*OH(I)+R(62,I)*O(I)+R(94,I)*OS(I)
PH2SO4(I)=R(71,I)*OH(I)*SO2(I)+R(83,I)*HO2(I)*SO2(I)
+PNHSO(I)
1 +R(11,I)*SO2(I)*O(I)
2 +R(120,I)*SO2(I)*CH3O2(I)
DH2SO4(I)=RN(7,I)
```

149 CONTINUE

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CHLOR

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DO 179 I=IANF,IEND,IDH
PHCL(I)=R(93,I)*CH2O(I)*CL(I)+D(28,I)*HOCL(I)+R(87,I)*CL(I)*CH4(I)
1 +R(85,I)*H2(I)*CL(I)+R(84,I)*HO2(I)*CL(I)
2 +R(52,I)*HNO4(I)*CL(I)+R(79,I)*OH(I)*CCL4(I)
3 +2.*R(191,I)*CL(I)*CH3CL(I)+R(186,I)*C2H6(I)*CL(I)
4 +R(183,I)*C2H2(I)*CL(I)+R(180,I)*C3H8(I)*CL(I)
5 +R(174,I)*CL(I)*HOCL(I)
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6      +R(121,I)*H2O2(I)*CL(I)+R(112,I)*HNO3(I)*CL(I)
DHCL(I)=R(72,I)*OH(I)+D(17,I) +RN(9,I)
1      +R(106,I)*O(I)+R(110,I)*OS(I)+R(118,I)*H(I)
PF12(I)=0.
DF12(I)=R(27,I)*OS(I)+R(77,I)*OH(I)+D(21,I)
PF11(I)=0.
DF11(I)=R(28,I)*OS(I)+R(78,I)*OH(I)+D(22,I)
PCCL4(I)=0.
DCCL4(I)=R(79,I)*OH(I)+D(23,I)+R(189,I)*OS(I)
PCH3CL(I)=0.
DCH3CL(I)=R(16,I)*O(I)+R(80,I)*OH(I)+D(24,I)+R(191,I)*CL(I)
PCHCL3(I)=0.
DCHCL3(I)=R(177,I)*OH(I)
PC2CL3(I)=0.
DC2CL3(I)=D(35,I)+R(178,I)*OH(I)

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C
C

KOULENSTOFF

```

PCO(I)=R(32,I)*O2(I)*CHO(I)+R(79,I)*OH(I)*CCL4(I)+D(19,I)*CH2O(I)
1      +D(18,I)*CO2(I)+D(13,I)*COS(I)+R(183,I)*CL(I)*C2H2(I)
2      +R(189,I)*OS(I)*CCL4(I)+R(62,I)*O(I)*COS(I)
3      +D(35,I)*C2CL3(I)+R(182,I)*OS(I)*C2H2(I)+R(172,I)*O(I)*C2H2(I)
4      +R(177,I)*OH(I)*CHCL3(I)
5      +R(107,I)*O(I)*CHO(I)
DCO(I)=R(73,I)*OH(I)+R(74,I)*OH(I)
1      +R(125,I)*CH3O(I)
PCO2(I)=R(73,I)*OH(I)*CO(I)+R(74,I)*OH(I)*CO(I)
1      +R(58,I)*COS(I)*OH(I)+R(94,I)*COS(I)*OS(I)
2      +R(125,I)*CH3O(I)*CO(I)
DCO2(I)=D(18,I)
PCH4(I)=0.
DCH4(I)=R(25,I)*OS(I)+R(26,I)*OS(I)+R(76,I)*OH(I)+R(87,I)*CL(I)
1      +R(108,I)*O(I)
PC2H6(I)=0.
DC2H6(I)=R(187,I)*OH(I)+R(186,I)*CL(I)+R(185,I)*OS(I)
PC2H2(I)=0.
DC2H2(I)=R(184,I)*OH(I)+R(183,I)*CL(I)+R(182,I)*OS(I)
1      +R(172,I)*O(I)
PC3H8(I)=0.
DC3H8(I)=R(181,I)*OH(I)+R(180,I)*CL(I)+R(179,I)*OS(I)

```

C

```

PDUM1(I)=0.
DDUM1(I)=1.D-17*O3(I)
PDUM2(I)=1.D-17*O3(I)*DUM1(I)
DDUM2(I)=D(19,I)+D(20,I)+RN(10,I)
PDUM3(I)=0.
DDUM3(I)=0.
PDUM4(I)=0.
DDUM4(I)=0.
PDUM5(I)=0.
DDUM5(I)=0.

```

179 CONTINUE

C
C
C
C

CHECK FOR H-, CL- AND S-ATOMS

```

ICHECK=IP(5)
IF (ICHECK.EQ.0) GOTO 300
NIX=NIX+1
I=30
IA=1+IDH*(20/IDH)
C*****DO 2099 I=IA,IEND,IDH
R11=R(11,I)*SO2(I)*O(I)

```

```

PX=PHODD(I)+2.*PH2(I)+2.*PH2O(I)+2.*PH2O2(I)+2.*PWSSR(I)+PHCL(I)+
1 PHNO3(I)+3.*PNH3(I)+2.*PHXS(I)+
2 4.*PCH4(I)+2.*PC2H2(I)+6.*PC2H6(I)+8.*PC3H8(I)+
3 PCHO(I)+3.*PCH3(I)+2.*PCH2O(I)+3.*PCH3O(I)+3.*PCH3O2(I)+
4 2.*(PH2SO4(I)-R11)+PCHCL3(I)+3.*PCH3CL(I)+
5 3.*PC2CL3(I)
DX=DHODD(I)*HODD(I)+2.*DH2(I)*H2(I)+2.*DH2O(I)*H2O(I)+
1 2.*DH2O2(I)*H2O2(I)+2.*DWSSR(I)*WSSR(I)+DHCL(I)*HCL(I)+
2 DHNO3(I)*HNO3(I)+
3 3.*DNH3(I)*ANH3(I)+2.*DHXS(I)*HXS(I)+
4 2.*DH2SO4(I)*H2SO4(I)+4.*DCH4(I)*CH4(I)+DCHCL3(I)*CHCL3(I)+
5 2.*DC2H2(I)*C2H2(I)+6.*DC2H6(I)*C2H6(I)+8.*DC3H8(I)*C3H8(I)+
6 DCHO(I)*CHO(I)+3.*DCH3(I)*CH3(I)+2.*DCH2O(I)*CH2O(I)+
7 3.*DCH3O(I)*CH3O(I)+3.*DCH3O2(I)*CH3O2(I)+
8 3.*DCH3CL(I)*CH3CL(I)+3.*DC2CL3(I)*C2CL3(I)
IJ=1
Y=PX-DX
X=(PX-DX)/PX
IF (DABS(X).GT.1.D-12) WRITE (9,1) NIX,I,IJ,X,Y,PX,DX
PX=PCLX(I)+3.*PF11(I)+2.*PF12(I)+4.*PCCL4(I)+PCH3CL(I)+
1 3.*PCHCL3(I)+3.*PC2CL3(I)+PHCL(I)
DX=DCLX(I)*CLX(I)+3.*DF11(I)*F11(I)+2.*DF12(I)*F12(I)
1 +4.*DCCL4(I)*CCL4(I)+DCH3CL(I)*CH3CL(I)+
2 3.*DCHCL3(I)*CHCL3(I)+3.*DC2CL3(I)*C2CL3(I)+
3 DHCL(I)*HCL(I)
IJ=2
Y=PX-DX
X=(PX-DX)/PX
IF (DABS(X).GT.1.D-12) WRITE (9,1) NIX,I,IJ,X,Y,PX,DX
PX=PSOX(I)+PHXS(I)+PH2SO4(I)+PCOS(I)
DX=DSOX(I)*SOX(I)+DHXS(I)*HXS(I)+DH2SO4(I)*H2SO4(I)+
* DCOS(I)*COS(I)
IJ=3
Y=PX-DX
X=(PX-DX)/PX
IF (DABS(X).GT.1.D-12) WRITE (9,1) NIX,I,IJ,X,Y,PX,DX
2099 CONTINUE
300 CONTINUE
RETURN
END

```

/*

```
//ICH301D5 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D5,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
C
C
C          DDD      5555
C          D  D      5
C          D  D      5  5
C          DDD      55
C
C *****
C *
C *      UNTERPROGRAMM: CALCULATION OF THE EQUATION SYSTEM
C *
C *****
C
C PURPOSE          : SOLVING THE MATRIX EQUATION DERIVED FROM
C                   THE DIFFERENTIAL EQUATION IN SPACE
C INPUT VIA CALL   : IO,N: FIRST AND LAST ALTITUDE
C                   IX: NUMBER OF COMPONENT TO BE CALCULATED
C                   NSED: SWITCH  =0: NO SEDIMENTATION
C                           =1: SEDIMENTATION INCLUDED
C INPUT VIA COMMON: EDD: EDDY DIFFUSION COEFFICIENT
C                   DZ: ALTITUDINAL SPACING
C                   AM: AIR CONCENTRATION  (=CX(I,40))
C                   PX: PRODUCTION RATES
C                   DX: DESTRUCTION FREQUENCIES
C                   XMR: MIXING RATIO AT GROUNDLEVEL
C                   PRD: PRODUCTION FLUX AT GROUNDLEVEL
C                   VDP: DEPOSITION VELOCITY
C OUTPUT VIA CALL  : X: MIXING RATIO OF SPECIES NO.IX
C
C      SUBROUTINE GAUSS (IO,N,IX,NSED,X)
C
C      IMPLICIT REAL *8 (A-H,O-Z)
C      COMMON /MET / EDD(0:99),TEMP(0:99),DZ
C      COMMON /CONC/ CX(0:99,0:63)
C      COMMON /TERME/ PX(0:99,2:63),DX(0:99,2:63),TT(0:99,2:33)
C      COMMON /BNDC/ XMR(33),PRD(33),VDP(33),X99(33)
C
C      DIMENSION A(0:99),B(0:99),C(0:99),D(0:99),AM(0:99),X(0:99),W(0:99)
C      EQUIVALENCE (AM(0),CX(0,0))
C
C      1000 FORMAT ('1')
C      2000 FORMAT (I5,1P, 5E12.2)
C
C      VSED(H)=-EXP(-6.12+1.95E-2*H+5.22E-3*H*H-8.31E-5*H**3
1      +3.92E-7*H**4)*NSED1
C
C      XMR(16)=CX(19,16)/AM(19)
C      NSED1=NSED
C      I1=IO+1
C      A(IO)=0.
C      DO 1 I=I1,N
C          A(I)=-(EDD(I)*AM(I)+EDD(I-1)*AM(I-1))/(2.*DZ*DZ)
C          C(I-1)=A(I)
C          B(I-1)=-(A(I-1)+C(I-1))+DX(I-1,IX)*AM(I-1)
1 CONTINUE
C      B(IO)=1.
C      C(IO)=0.
C      E1=1./(3.+2.*DZ/EDD(IO)*VDP(IX))
```

```
IF (XMR(IX).NE.0.) E1=0.
NM1=N-1
NM2=N-I0-1
I3=I0+2
D(I0)=-E1*4.
W(I0)=2.*DZ/(EDD(I0)*AM(I0))*PRD(IX)*E1+XMR(IX)
H=I0
V=VSED(H-.5)/(2.*DZ)
VA=-V*AM(I0)
VB=+V*AM(I0+1)
V=VSED(H+.5)/(2.*DZ)
VC=+V*AM(I0+2)
VB=VB-V*AM(I0+1)
XN=(B(I0+1)+VB)-(A(I0+1)+VA)*D(I0)
D(I0+1)=((C(I0+1)+VC)-(A(I0+1)+VA)*E1)/XN
W(I0+1)=(PX(I0+1,IX)-(A(I0+1)+VA)*W(I0))/XN
DO 9 I=I3,NM1
NSED1=(1-I/50)*NSED
H=I-1
VA=-V*AM(I-1)
VB=+V*AM(I)
V=VSED(H+.5)/(2.*DZ)
VC=+V*AM(I+1)
VB=VB-V*AM(I)
XN=(B(I)+VB)-(A(I)+VA)*D(I-1)
D(I)=(C(I)+VC)/XN
W(I)=(PX(I,IX)-(A(I)+VA)*W(I-1))/XN
9 CONTINUE
X(N)=X99(N)
DO 19 I=NM1,I1,-1
X(I)=W(I)-D(I)*X(I+1)
19 CONTINUE
X(I0)=W(I0)-D(I0)*X(I0+1)-E1*X(I0+2)
RETURN
END
```

/*

//ICH301D6 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)

/*PASSWORD MODEL

/*ROUTE PRINT MVS

// EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D6,

// PARM.C='MAP,XREF,OPTIMIZE(2)'

//SYSUT5 DD UNIT=TEMP,SPACE=(6400,90)

//C.SYSIN DD *

C			
C		DDD	666
C		D D	6
C		D D	6 6
C		DDD	666

 *
 * SUBROUTINE FOR TRANSPORT *
 *

C PURPOSE : CALCULATION OF THE TRANSPORT TERM FOR THE
 C TIME-DEPENDENT VERSIONS
 C INPUT VIA CALL : IS : SWITCH =1: CALCULATION OF AVERAGING FACTOR
 C =2: NORMALIZED STEADY-STATE FLUX
 C =3: TRANSPORT AVERAGED OVER TIME-STEP
 C IDH : ALTITUDE STEP
 C DT : TIME STEP
 C INPUT VIA COMMON: C : CONCENTRATION PROFILES OF CONSTITUENTS
 C P,D : PRODUCTION RATES AND DESTRUCTION FREQUENCIES
 C EDD : EDDYDIFFUSION COEFFICIENT
 C DZ : ALTITUDINAL SPACING
 C PRD : PRODUCTION RATES AT GROUND LEVEL
 C VDP : DEPOSITION VELOCITIES
 C OUTPUT VIA COMMON:TT : TRANSPORT TERM

SUBROUTINE TRANS (IS,IDH,IEND,DT)

IMPLICIT REAL*8 (A-H,O-Z)

COMMON

COMMON /CONC / C(0:99,0:63)
 COMMON /TERME/ P(0:99,2:63),D(0:99,2:63),TT(0:99,2:33)
 COMMON /MET / EDD(0:99),TEMP(0:99),DZ
 COMMON /BNDC / XMR(33),PRD(33),VDP(33),X99(33)

DIMENSION

DIMENSION AM(0:99),FL(0:99,2:33),X(0:99),FAK(99),RKM(0:99)
 EQUIVALENCE (AM(0),C(0,0))
 CALL MASKE

DATA

DATA FL /3200*0./
 ISTART=0
 JEND=33
 DZZ=DZ*DZ
 NSED=0
 IENDG=99

```

C      GOTO (100,200,300),IS
C
C      CALCULATION OF THE AVERAGING FACTOR
100 CONTINUE
    RKM(0)=EDD(0)*AM(0)
    DO 109 I=1,IEND
        RKM(I)=DSQRT(EDD(I-1)*AM(I-1)*EDD(I)*AM(I))
        ALPHA=2.*RKM(I)/(DZZ*AM(I))
        FAK(I)=(1.-DEXP(-ALPHA*DT))/(ALPHA*DT)
109 CONTINUE
    RETURN
C
C      NORMALIZED FLUX FOR INFINITY FROM STEADY-STATE
200 CONTINUE
    DO 299 J=2,JEND
        IA=ISTART
        IF (J.NE.16) GOTO 203
        IA=20
        XMR(16)=5.D-6
203    CALL GAUSS (IA,IENDG,J,NSED,X)
        IF (X(IA).EQ.0.DO) GOTO 299
        CO=X(IA)*AM(IA)
        DO 209 I=IA+1,IEND
            FL(I,J)=-RKM(I)*(X(I)-X(I-1))/DZ/CO
209    CONTINUE
        FL(IA,J)=-RKM(IA)*(-3.*X(IA)+4.*X(IA+1)-X(IA+2))/(2.*DZ*CO)
        DO 219 I=IA,IEND
            TT(I,J)=- (FL(I+1,J)-FL(I,J))/DZ*C(IA,J)
219    CONTINUE
        TT(IA,J)=TT(IA,J)/2.
299 CONTINUE
    RETURN
C
C      TRANSPORT AVERAGED OVER TIME-STEP DT
300 CONTINUE
    DO 399 J=2,JEND
        IF (J.EQ.17) GOTO 399
        IA=ISTART
        IF (J.EQ.16) IA=20
        PHI0=-RKM(IA+1)*(C(IA+1,J)/AM(IA+1)-C(IA,J)/AM(IA))/DZ
        PHIUN=FL(IA+1,J)*C(IA,J)
        PHI0=PHIUN+(PHI0-PHIUN)*FAK(IA+1)
        PHIU=PRD(J)-VDP(J)*C(IA,J)
        IF (XMR(J).NE.0.DO) PHIU=-RKM(IA)*(-3.*C(IA,J)/AM(IA)+4.*
*          C(IA+1,J)/AM(IA+1)-C(IA+2,J)/AM(IA+2))/(2.*DZ)
        TT(IA,J)=((PHIU+FL(IA,J)*C(IA,J))/2.-PHI0)/DZ
        PHIU=PHI0
        DO 309 I=IA+1,IEND
            PHI0=-RKM(I+1)*(C(I+1,J)/AM(I+1)-C(I,J)/AM(I))/DZ
            PHIUN=FL(I+1,J)*C(IA,J)
            PHI0=PHIUN+(PHI0-PHIUN)*FAK(I+1)
            TT(I,J)=- (PHI0-PHIU)/DZ
            PHIU=PHI0
309    CONTINUE
399 CONTINUE
C
    RETURN
1 FORMAT (1X,2I10,1P,10E10.2)
END

```

/*

```
//ICH301D7 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301D7,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
C
C
C          DDD      7777
C          D  D      7
C          D  D      7
C          DDD      7
C
C *****
C *
C *   UNTERPROGRAMM ;   DIFFERENTIAL EQATION IN TIME
C *
C *****
C
C PURPOSE :      SOLUTION OF THE TIME-DEPENDENT DIFFERENTIAL EQUATION
C INPUT VIA CALL   : DT : TIME STEP
C                   IDH : ALTITUDE STEP
C                   IS  : SWITCH=1: CALCULATION OF NORMALISATION FACTOR
C                       =2: SOLUTION OF THE DIFFERENTIAL EQUATION
C                       =3: AS 2 PLUS ADDITION OF GROUND FLUX
C INPUT VIA COMMON : C   : OLD CONCENTRATION PROFILES OF THE COMPONENTS
C                   P,D : PRODUCTION RATES AND DESTRUCTION FREQUENCIES
C                   TT  : TRANSPORT TERM TO BE ADDED TO P
C                   EDD : EDDYDIFFUSION COEFFICIENT
C                   DZ  : ALTITUDE STEP IN KM
C                   XMR : MIXING RATIO AT GROUND LEVEL
C                   PRD : PRODUCTION FLUX AT GROUND LEVEL
C                   VDP : DEPOSITION VELOCITY
C                   TAU : TIME SHIFT FACTOR
C OUTPUT VIA COMMON : C   : NEW CONCENTRATION PROFILES OF THE COMPONENTS
C
C   SUBROUTINE EULER (DTT,IDH,IEND,IS)
C   =====
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C
C   COMMON
C   -----
C   COMMON /CONC/ C1(0:99,0:33),C2(0:99,1:30)
C   COMMON /TERME/ P1(0:99,2:33),P2(0:99,1:30),
C *           D1(0:99,2:33),D2(0:99,1:30),TT(0:99,2:33)
C   COMMON /MET/ EDD(0:99),TEMP(0:99),DZ
C   COMMON /BNDC/ XMR(33),PRD(33),VDP(33),X99(33)
C   COMMON /ZENITH/ ALPHA,BETA,TAU(0:99)
C   COMMON /ISWTCH/ IP(12)
C
C   DECLARE
C   -----
C
C   DIMENSION FAK(0:15)
C   DATA FAK /16*0./
C   CALL MASKE
C   IANF=0
C   ISUB=IP(4)
C
C   GOTO (100,200,200),IS
C
C   NORMALISATION FACTOR
```

```

C -----
C
100 CONTINUE
    SIGMA=SQRT(EDD(5)*DTT*2.)
    F=C1(1,0)/4.
    DO 19 I=0,14
        F=F+SQRT(C1(I,0)*C1(I+1,0))*0.5*DEXP(-((I+0.5)*DZ/SIGMA)**2)
        F=F+C1(I+1,0)*0.5*DEXP(-(DZ*(I+1)/SIGMA)**2)
19    CONTINUE
    DO 18 I=0,15
        FAK(I)=C1(I,0)/F*DEXP(-(DZ*I/SIGMA)**2)*DTT/DZ
18    CONTINUE
    FAK(0)=FAK(0)/2.
    RETURN

C
C EULER SOLUTION FOR STABLE CONSTITUENTS
C -----
C
200 CONTINUE
    DO 29 J=2,33
        IA=IANF
        IF (XMR(J).NE.0.) IA=IANF+1
        IF (J.EQ.16) IA=20
        IF (J.EQ.ISUB) GOTO 29
        DO 29 I=IA,IEND,IDH
            DT=DTT*TAU(I)
            X=D1(I,J)*DT
            IF (X.LT.1.D-20) THEN
                C1(I,J)=C1(I,J)+(P1(I,J)+TT(I,J))*DT
            ELSE
                Y=(P1(I,J)+TT(I,J))/D1(I,J)
                C1(I,J)=Y+(C1(I,J)-Y)*EXP(-X)
            ENDIF
            C1(I,J)=DMAX1(C1(I,J),0.D0)
29    CONTINUE
    GOTO (300,400,300),IS

C
C ADDITION OF GROUND-FLUX
C -----
C
300 DO 39 J=2,33
    IF (XMR(J).NE.0.) GOTO 39
    DO 39 I=0,15
        X=D1(I,J)*DTT
        C1(I,J)=C1(I,J)+(PRD(J)-VDP(J)*C1(0,J))*FAK(I)*DEXP(-X)
        C1(I,J)=DMAX1(C1(I,J),0.D0)
39    CONTINUE
    RETURN

C
C EULER SOLUTION FOR RADICALS
C -----
C
400 DO 49 J=1,30
    DO 49 I=IANF,IEND,IDH
        DT=DTT*TAU(I)
        X=D2(I,J)*DT
        IF (X.LT.1.D-10) THEN
            C2(I,J)=C2(I,J)+P2(I,J)*DT
        ELSE
            Y=P2(I,J)/D2(I,J)
            C2(I,J)=Y+(C2(I,J)-Y)*EXP(-X)
        ENDIF
        C2(I,J)=DMAX1(C2(I,J),0.D0)
49    CONTINUE

```

```
C
      RETURN
1000  FORMAT (10F10.2)
2000  FORMAT (1P,10E12.3)
      END
/*
```

```
//ICH301E1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301E1,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          EEEE      1
C          E      1 1
C          E      1
C          EEEE      1
C
C *****
C *
C *      UNTERPROGRAMM: OUTPUT OF CONCENTRATIONS AND
C *      MIXING RATIOS
C *
C *****
C
C PURPOSE          : OUTPUT OF CONCENTRATION- AND/OR MIXING RATIO-
C                   PROFILES AT A SPECIFIC TIME
C INPUT VIA CALL   : XT: SPECIFIC TIME
C                   IS: SWITCH FOR OUTPUT: 0=CONCENTRATIONS
C                                     1=CONCENTR.+MIX.RATIOS
C                                     2=MIXING RATIOS
C
C                   ISP: ALTITUDINAL STEP
C                   ITYP: TYP OF HEADING
C INPUT VIA COMMON : C1,C2: CONCENTRATION PROFILES
C OUTPUT ON PRINTER: CONCENTRATIONS AND/OR MIXING RATIOS
```

```
C      SUBROUTINE OUTPT (XT,IS,ISP,IJ,ITYP)
```

```
C      IMPLICIT REAL*8 (A-H,O-Z)
```

```
C      COMMON /CONC/ C1(0:99,0:33),C2(0:99,1:30)
```

```
C      DECLARE
```

```
C      -----
C      EQUIVALENCE          (AM      (0), C1(0, 0)),( O2      (0), C1(0, 1)),
1( ODD      (0), C1(0, 2)),(ANODD (0), C1(0, 3)),( HODD      (0), C1(0, 4)),
2( SOX      (0), C1(0, 5)),( HXS      (0), C1(0, 6)),( CLX      (0), C1(0, 7)),
3( CW       (0), C1(0, 8)),( DUM1      (0), C1(0, 9)),( DUM2      (0), C1(0,10)),
4(AN2O      (0), C1(0,11)),(ANH3      (0), C1(0,12)),(ANH4      (0), C1(0,13)),
5( HNO3      (0), C1(0,14)),( H2       (0), C1(0,15)),( H2O      (0), C1(0,16)),
6( WSSR      (0), C1(0,17)),( H2O2      (0), C1(0,18)),( H2SO4(0), C1(0,19)),
7( CO5      (0), C1(0,20)),( CO       (0), C1(0,21)),( CO2      (0), C1(0,22)),
8( CH4      (0), C1(0,23)),( C2H2      (0), C1(0,24)),( C2H6      (0), C1(0,25)),
9( C3H8      (0), C1(0,26)),( F11      (0), C1(0,27)),( F12      (0), C1(0,28)),
A( CCL4      (0), C1(0,29)),( CH3CL(0), C1(0,30)),( CHCL3(0), C1(0,31)),
B( C2CL3(0), C1(0,32)),( HCL      (0), C1(0,33))
```

```
C      EQUIVALENCE          ( O      (0), C2(0, 1)),
1( OS       (0), C2(0, 2)),( O3       (0), C2(0, 3)),(AN      (0), C2(0, 4)),
2(ANO      (0), C2(0, 5)),(ANO2      (0), C2(0, 6)),(ANO3      (0), C2(0, 7)),
3(AN2O5      (0), C2(0, 8)),( HNO2      (0), C2(0, 9)),( HNO4      (0), C2(0,10)),
4( H        (0), C2(0,11)),( OH        (0), C2(0,12)),( HO2      (0), C2(0,13)),
5( SO       (0), C2(0,14)),( SO2      (0), C2(0,15)),( HS       (0), C2(0,16)),
6( H2S      (0), C2(0,17)),( CL       (0), C2(0,18)),( CLO      (0), C2(0,19)),
7( CL2      (0), C2(0,20)),( HOCL      (0), C2(0,21)),( CLNO3(0), C2(0,22)),
8( CHO      (0), C2(0,23)),( CH3      (0), C2(0,24)),( CH2O      (0), C2(0,25)),
9( CH3O      (0), C2(0,26)),( CH3O2(0), C2(0,27)),( DUM3      (0), C2(0,28)),
A( DUM4      (0), C2(0,29)),( DUM5      (0), C2(0,30))
```

```

C
C  DIMENSIONEN
C  -----
C
REAL *8 AM      (0:99), O2      (0:99), ODD      (0:99), ANODD (0:99),
1      HODD (0:99), SOX      (0:99), HXS      (0:99), CLX      (0:99),
2      CW      (0:99), DUM1 (0:99), DUM2 (0:99), AN2O      (0:99),
3      ANH3      (0:99), ANH4      (0:99), HNO3      (0:99), H2      (0:99),
4      H2O      (0:99), WSSR      (0:99), H2O2      (0:99), H2SO4(0:99),
5      COS      (0:99), CO      (0:99), CO2      (0:99), CH4      (0:99),
6      C2H2      (0:99), C2H6      (0:99), C3H8      (0:99), F11      (0:99),
7      F12      (0:99), CCL4      (0:99), CH3CL(0:99), CHCL3(0:99),
8      C2CL3(0:99), HCL      (0:99)
REAL *8 O      (0:99), OS      (0:99), O3      (0:99), AN      (0:99),
1      ANO      (0:99), ANO2      (0:99), ANO3      (0:99), AN2O5 (0:99),
2      HNO2      (0:99), HNO4      (0:99), H      (0:99), OH      (0:99),
3      HO2      (0:99), SO      (0:99), SO2      (0:99), HS      (0:99),
4      H2S      (0:99), CL      (0:99), CLO      (0:99), CL2      (0:99),
5      HOCL      (0:99), CLNO3(0:99), CHO      (0:99), CH3      (0:99),
6      CH2O      (0:99), CH3O      (0:99), CH3O2(0:99), DUM3      (0:99),
7      DUM4      (0:99), DUM5      (0:99)
CHARACTER*8 TEX,TEXT(5)

C
C  FORMATE
1 FORMAT (I5,1P,14E9.2)
2 FORMAT(I1,30X,'CONCENTRATION OF TRACE CONSTITUENTS      IN MOLECULES
  1 PER CM3',20X,F5.0,A8/)
3 FORMAT(I1,50X,'VOLUME MIXING RATIOS',38X,F5.0,A8/)
4 FORMAT (' ALT.  AIR      O2      O      O3      O(1D)      ODD
  1 DUMMY1 DUMMY2 DUMMY3 DUMMY4 DUMMY5')
5 FORMAT (' ALT.  CL      CLO      CLX      CLNO3      HOCL      HCL
  1 CL2      F 11      F 12      CH3CL      CHCL3      CCL4      CH3CCL3
  2 SUM CL')
6 FORMAT (' ALT.  H      OH      HO2      HODD      H2O2      H2
  1 H2O      WASSER SUM H')
7 FORMAT (' ALT.  N      NO      NO2      NO3      HNO2      N2O5
  1 HO2NO2 NODD      HNO3      N2O      NH3      NH4OH')
8 FORMAT (' ALT.  CO      CO2      CH4      CH2O      CH3      CHO
  1 CH3O      CH3O2      CW      C2H6      C2H2      C3H8')
9 FORMAT (' ALT.  SO      SO2      SOX      COS      HS      H2S
  1 HXS      H2SO4      SUM S')

C
DATA TEXT/'STEP      ', 'UHR      ', 'START      ', 'END      ', 'JAHR      '/

C
CALL MASKE

C
IF (ITYP.EQ.1) TEX=TEXT(1)
IF (ITYP.EQ.2) TEX=TEXT(5)
IF (ITYP.EQ.3) TEX=TEXT(2)
IF (ITYP.EQ.0) TEX=TEXT(3)
IF (ITYP.GE.8) TEX=TEXT(4)

C
KONZENTRATIONEN
II=0
10 NZZ=1
NRZ=7+(IJ-II)/ISP
NSZ=1
IF (IS.EQ.2) GOTO 20
WRITE(6,2) NSZ,XT,TEX
WRITE(6,4)
DO 11 I=II,IJ,ISP
11 WRITE (6,1) I,AM(I),O2(I),O(I),O3(I),OS(I),ODD(I),DUM1(I),
  1 DUM2(I),DUM3(I),DUM4(I),DUM5(I)
WRITE(6,4)

```

```

      NSZ=0
      NZZ=NZZ+1
      IF (NZZ*NRZ.LT.70) GOTO 120
      NSZ=1
      NZZ=0
120  WRITE(6,2) NSZ,XT,TEX
      WRITE(6,5)
      DO 12 I=II,IJ,ISP
          SCL=CLX(I)+3.*F11 (I)+2.*F12 (I)+CH3CL(I)+4.*CCL4(I)+HCL(I)
          1 +CL2(I)+3.*C2CL3(I)+HOCL(I)+CLNO3(I)+3.*CHCL3(I)
12  WRITE (6,1) I,CL(I),CLO(I),CLX(I),CLNO3(I),HOCL(I),HCL(I),CL2(I)
          1 ,F11(I),F12(I),CH3CL(I),CHCL3(I),CCL4(I),C2CL3(I),SCL
      WRITE (6,5)
      NSZ=0
      NZZ=NZZ+1
      IF (NZZ*NRZ.LT.70) GOTO 130
      NSZ=1
      NZZ=0
130  WRITE(6,2) NSZ,XT,TEX
      WRITE(6,6)
      DO 13 I=II,IJ,ISP
          SH=HODD(I)+H2O2(I)*2.+H2(I)*2.+H2O(I)*2.+WSSR(I)*2.+CH4(I)*4.+
          1 CH2O(I)*2.+HOCL(I)+HNO4(I)+HNO2(I)
13  WRITE (6,1) I,H(I),OH(I),HO2(I),HODD(I),H2O2(I),H2(I),H2O(I),
          1 WSSR(I) ,SH
      WRITE(6,6)
      NSZ=0
      NZZ=NZZ+1
      IF (NZZ*NRZ.LT.70) GOTO 140
      NSZ=1
      NZZ=0
140  WRITE(6,2) NSZ,XT,TEX
      WRITE(6,7)
      DO 14 I=II,IJ,ISP
14  WRITE (6,1) I,AN(I),ANO(I),ANO2(I),ANO3(I),HNO2(I),AN2O5(I),
          1 HNO4(I),ANODD(I),HNO3(I),AN2O(I),ANH3(I),ANH4(I)
      WRITE(6,7)
      NSZ=0
      NZZ=NZZ+1
      IF (NZZ*NRZ.LT.70) GOTO 150
      NSZ=1
      NZZ=0
150  WRITE(6,2) NSZ,XT,TEX
      WRITE(6,8)
      DO 15 I=II,IJ,ISP
15  WRITE (6,1) I,CO(I),CO2(I),CH4(I),CH2O(I),CH3(I),CHO(I),CH3O(I),
          1 CH3O2(I),CW(I),C2H6(I),C2H2(I),C3H8(I)
      WRITE(6,8)
      NSZ=0
      NZZ=NZZ+1
      IF (NZZ*NRZ.LT.70) GOTO 160
      NSZ=1
      NZZ=0
160  WRITE(6,2) NSZ,XT,TEX
      WRITE(6,9)
      DO 16 I=II,IJ,ISP
          SS=SOX(I)+COS(I)+HXS(I)+H2SO4(I)
16  WRITE (6,1) I,SO(I),SO2(I),SOX(I),COS(I),HS(I),H2S(I),
          1 HXS(I),H2SO4(I),SS
      WRITE(6,9)
C
C  MISCHUNGSVERHAELTNISSE
20  CONTINUE
```

```

IF (IS.EQ.0) RETURN
NSZ=1
NZZ=1
WRITE(6,3) NSZ,XT,TEX
WRITE(6,4)
DO 21 I=II,IJ,ISP
U1=AM(I)
U2=O2(I)/AM(I)
U3=O(I)/AM(I)
U4=O3(I)/AM(I)
U5=OS(I)/AM(I)
U6=ODD(I)/AM(I)
U7=DUM1(I)/AM(I)
U8=DUM2(I)/AM(I)
U9=DUM3(I)/AM(I)
U10=DUM4(I)/AM(I)
U11=DUM5(I)/AM(I)
21 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9,U10,U11
WRITE(6,4)
NSZ=0
NZZ=NZZ+1
IF (NZZ*NRZ.LT.70) GOTO 220
NSZ=1
NZZ=0
220 WRITE(6,3) NSZ,XT,TEX
WRITE(6,5)
DO 22 I=II,IJ,ISP
U1=CL(I)/AM(I)
U2=CLO(I)/AM(I)
U3=CLX(I)/AM(I)
U4=CLNO3(I)/AM(I)
U5=HOCL(I)/AM(I)
U6=HCL (I)/AM(I)
U7=CL2 (I)/AM(I)
U8=F11 (I)/AM(I)
U9=F12 (I)/AM(I)
U10=CH3CL(I)/AM(I)
U11=CHCL3(I)/AM(I)
U12=CCL4(I)/AM(I)
U13=C2CL3(I)/AM(I)
U14=U3+U4+U5+U6+2.*U7+3.*U8+2.*U9+U10+3.*U11+4.*U12+3.*U13
22 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9,U10,U11,U12,U13,U14
WRITE(6,5)
NSZ=0
NZZ=NZZ+1
IF (NZZ*NRZ.LT.70) GOTO 230
NSZ=1
NZZ=0
230 WRITE(6,3) NSZ,XT,TEX
WRITE(6,6)
DO 23 I=II,IJ,ISP
U1=H(I)/AM(I)
U2=OH(I)/AM(I)
U3=HO2(I)/AM(I)
U4=HODD(I)/AM(I)
U5=H2O2(I)/AM(I)
U6=H2(I)/AM(I)
U7=H2O(I)/AM(I)
U8=WSSR(I)/AM(I)
SH=HODD(I)+H2O2(I)*2.+H2(I)*2.+H2O(I)*2.+WSSR(I)*2.+CH4(I)*4.+
1 CH2O(I)*2.+HOCL(I)+HNO4(I)+HNO2(I)
U9=SH/AM(I)
23 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9

```

```
WRITE(6,6)
NSZ=0
NZZ=NZZ+1
IF (NZZ*NRZ.LT.70) GOTO 240
NSZ=1
NZZ=0
240 WRITE(6,3) NSZ,XT,TEX
WRITE(6,7)
DO 24 I=II,IJ,ISP
U1=AN(I)/AM(I)
U2=ANO(I)/AM(I)
U3=ANO2(I)/AM(I)
U4=ANO3(I)/AM(I)
U5=HNO2(I)/AM(I)
U6=AN2O5(I)/AM(I)
U7=HNO4(I)/AM(I)
U8=ANODD(I)/AM(I)
U9=HNO3(I)/AM(I)
U10=AN2O(I)/AM(I)
U11=ANH3(I)/AM(I)
U12=ANH4(I)/AM(I)
24 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9,U10,U11,U12
WRITE(6,7)
NSZ=0
NZZ=NZZ+1
IF (NZZ*NRZ.LT.70) GOTO 250
NSZ=1
NZZ=0
250 WRITE(6,3) NSZ,XT,TEX
WRITE(6,8)
DO 25 I=II,IJ,ISP
U1=CO(I)/AM(I)
U2=CO2(I)/AM(I)
U3=CH4(I)/AM(I)
U4=CH2O(I)/AM(I)
U5=CH3(I)/AM(I)
U6=CHO(I)/AM(I)
U7=CH3O(I)/AM(I)
U8=CH3O2(I)/AM(I)
U9=CW(I)/AM(I)
U10=C2H6(I)/AM(I)
U11=C2H2(I)/AM(I)
U12=C3H8(I)/AM(I)
25 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9,U10,U11,U12
WRITE(6,8)
NSZ=0
NZZ=NZZ+1
IF (NZZ*NRZ.LT.70) GOTO 260
NSZ=1
NZZ=0
260 WRITE(6,3) NSZ,XT,TEX
WRITE(6,9)
DO 26 I=II,IJ,ISP
U1=SO(I)/AM(I)
U2=SO2(I)/AM(I)
U3=SOX(I)/AM(I)
U4=COS(I)/AM(I)
U5=HS(I)/AM(I)
U6=H2S(I)/AM(I)
U7=HXS(I)/AM(I)
U8=H2SO4(I)/AM(I)
U9=U3+U4+U7+U8
26 WRITE (6,1) I ,U1,U2,U3,U4,U5,U6,U7,U8,U9
```

```
      WRITE(6,9)
C
99  RETURN
END
/*
```

```
//ICH301E2 JOB (324,035430),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301E2,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C          MEMBER AUF OBJECT BRINGEN      EEEE      22
C          E      2  2
C          E      2
C          EEEE      2222
C
C      *****
C      *
C      *      UNTERPROGRAMM HOEPRO  HOEHENPROFIL      11.2.76      *
C      *
C      *****
C
C      SUBROUTINE HOEPRO (IS,AM,W1,W2,W3,W4,TEXT,IN,IX)
C      REAL*8 AM,W1,W2,W3,W4,XN,EX
C      DIMENSION W1(1),W2(1),W3(1),W4(1),ALT(100),TEXT(8),W(100,4),XS(4)
C      DIMENSION X(100),YS(4),AM(100)
C
C      L=2
C      M=4
C      N=60
C      XM=IN
C      DX=FLOAT(IX)/30.
C      XMAX=IN+IX
C
C      GOTO (5,3,5),IS
C
C      MIXING RATIO VS HEIGHT
C      3 DO 4 I=1,N
C        ALT(I)=I-1
C        W(I,1)=W1(I)/AM(I)*1.D6
C        W(I,2)=W2(I)/AM(I)*1.D6
C        W(I,3)=W3(I)/AM(I)*1.D6
C        W(I,4)=W4(I)/AM(I)*1.D6
C      4 CONTINUE
C      GOTO 7
C
C      CONCENTRATION OR PHOTODISSOCIATION COEFFICIENT VS HEIGHT
C      5 DO 6 I=1,N
C        ALT(I)=I-1
C        W(I,1)=W1(I)
C        W(I,2)=W2(I)
C        W(I,3)=W3(I)
C        W(I,4)=W4(I)
C      6 CONTINUE
C
C      7 ALT(N+1)=0.
C        ALT(N+2)=3.
C        DO 19 J=1,M
C          DO 19 I=1,N
C            GOTO (12,11),L
C      11 IF (W(I,J).LE.0.) W(I,J)=1.E-70
C        W(I,J)=ALOG10(W(I,J))
C      12 W(I,J)=AMAX1(W(I,J),XM)
C        W(I,J)=AMIN1(W(I,J),XMAX)
C      19 CONTINUE
C        DO 29 J=1,M
C          IJ=J*N /5
C          YS(J)=ALT(IJ)/3.
C      29 XS(J)=(W(IJ,J) -XM)/DX
```

```
C      GOTO (31,34,37),IS
C
C      CONCENTRATION VS HEIGHT
31 CONTINUE
   GOTO (32,33),L
32 CALL ACHSE (0.,0.,'CONCENTRATION/ CM-3',-19 ,30.,0.,XM,DX)
   CALL ACHSE (0.,20.,' ',1,30.,0.,XM,DX)
   GOTO 53
33 DXX=1./DX
   CALL LACHS (0.,0.,'CONCENTRATION/ CM-3',-19 ,30.,0.,XM,DXX)
   CALL LACHS (0.,20.,' ',1,30.,0.,XM,DXX)
   GOTO 53
C
C      MIXING RATIO VS HEIGHT
34 CONTINUE
   GOTO (35,36),L
35 CALL ACHSE (0.,0.,'VOLUME MIXING RATIO/ PPM',-24 ,30.,0.,XM,DX)
   CALL ACHSE (0.,20.,' ',1,30.,0.,XM,DX)
   GOTO 53
36 DXX=1./DX
   CALL LACHS (0.,0.,'VOLUME MIXING RATIO/ PPM',-24 ,30.,0.,XM,DXX)
   CALL LACHS (0.,20.,' ',1,30.,0.,XM,DXX)
   GOTO 53
C
C      PHOTODISSOCIATION COEFFICIENT VS HEIGHT
37 CONTINUE
   GOTO (38,39),L
38 CALL ACHSE (0.,0.,'PHOTODISSOCIATION COEFFICIENT IN S-1',-36,30.,0
* .,XM,DX)
   CALL ACHSE (0.,20.,' ',1,30.,0.,XM,DX)
   GOTO 53
39 DXX=1./DX
   CALL LACHS (0.,0.,'PHOTODISSOCIATION COEFFICIENT IN S-1',-36,30.,0
* .,XM,DXX)
   CALL LACHS (0.,20.,' ',1,30.,0.,XM,DXX)
53 CALL ACHSE (0.,0.,'ALTITUDE/ KM',12,20.,90.,0.,3.)
   CALL ACHSE (30.,0.,' ',-1,20.,90.,0.,3.)
C
C      ZEICHNEN UND BESCHRIFTEN DER KURVEN
   X(N+1)=XM
   X(N+2)=DX
   K=1
   DO 59 J=1,M
   DO 55 I=1,N
55 X(I)=W(I,J)
   CALL LINIE (X,ALT,N,1,0,0)
   CALL SYMBL (XS(J),YS(J),.5,TEXT(K),0.,4)
   IF (IS.NE.3) GOTO 58
C
C      PHOTODISSOCIATION COEFFICIENT
   CALL SYMBL (999.0,999.0,.5,TEXT(K+1),0.,4)
   K=K+1
58 K=K+1
59 CONTINUE
C
   CALL FRAMAD
   RETURN
   END
/*
```

```
//ICH301E3 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301E3,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
```

```
C
C
C          EEEE      333
C          E_        3
C          E         3
C          EEEE      333
```

```
C *****
C *                               *
C *   OUTPUT FOR LONG-TERM VARIATION   *
C *                               *
C *****
```

```
C
C
C      SUBROUTINE OUTLTM (K,IS)
```

```
C
C
C      COMMON
C      -----
```

```
C
C      COMMON /CONC/ X1,X2
C      COMMON /ISO/ Y
```

```
C
C      DECLARE
C      -----
```

```
C
C      REAL*8 X1(0:99,0:33),X2(0:99,1:30),Y(50,20,65)
C      DIMENSION SUBST1(33),SUBST2(30),SUBST(65)
C      EQUIVALENCE (SUBST(1),SUBST1(1)),(SUBST(34),SUBST2(1))
```

```
C
C      DATA
C      ----
```

```
C
C      DATA SUBST1/
C      1'O2 ','O ODD','N ODD','H ODD','SOX ','HXS ','CLX ','CW ','DUM1',
C      2'DUM2','N2O ','NH3 ','NH4+','HNO3','H2 ','H2O ','WSSR','H2O2',
C      3'HSO4','COS ','CO ','CO2 ','CH4 ','C2H2','C2H6','C3H8','F11 ',
C      4'F12 ','CCL4','C3CL','CCL3','C2CL','HCL '/
C      DATA SUBST2/
C      1'O ','OS ','O3 ','N ','NO ','NO2 ','NO3 ','N2O5','HNO2',
C      2'HNO4','H ','OH ','HO2 ','SO ','SO2 ','HS ','H2S ','CL ',
C      3'ClO ','CL2 ','HOCL','CLNO','CHO ','CH3 ','CH2O','CH3O','CHO2',
C      4'DUM3','DUM4','DUM5'/
C      IEND=65
```

```
C
C      IF (IS.NE.1) GOTO 200
C      DO 18 J=1,33
C      DO 18 I=0,IEND,5
C      IO=I/5+1
C      Y(K,IO,J)=X1(I,J)/X1(I,0)
18  CONTINUE
C      DO 19 J=1,30
C      DO 19 I=0,IEND,5
C      IO=I/5+1
C      Y(K+33,IO,J)=X2(I,J)/X1(I,0)
19  CONTINUE
C      RETURN
```

C

```
200 IF (IS.NE.2) RETURN
      DO 29 J0=1,63,2
        WRITE (6,2001)
        DO 29 J=J0,J0+1
          WRITE (6,2002) SUBST(J),((IX),IX=1,IEND,5)
          DO 29 KX=1,K
            WRITE (6,2003) KX,(Y(KX,I0,J),I0=1,14)
29      CONTINUE
      RETURN
```

C

```
2001 FORMAT ('1',40X,'VOLUME MIXING RATIOS')
2002 FORMAT (/5X,A4/'OJAHR ',I5,13I9,'KM'/)
2003 FORMAT (I6,1P,14E9.2)
      END
```

/*

```
//ICH301E4 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301E4,
//      PARM.C='MAP,XREF,OPTIMIZE(2)'
//C.SYSIN DD *
C
C
C          EEEE      4  4
C          E      4  4
C          E      444444
C          EEEE      4
C
C *****
C *
C *      OUTPUT FOR DIURNAL VARIATION
C *
C *****
C
C PURPOSE          : OUTPUT ROUTINE FOR THE DIURNAL VARIATION VERSION
C INPUT VIA CALL   : K : TIME INDEX
C                   IDH: ALTITUDINAL STEP
C                   IS : SWITCH      =1: COLLECTING DATA
C                                   =2: OUTPUT OF DATA
C                                   =3: DATA FOR BASELINE
C INPUT VIA COMMON : C : CONCENTRATION PROFILES
C                   TAU: TIME SHIFT FACTOR
C OUTPUT ON PRINTER: Y : MIXING RATIOS AT DIFFERENT TIMES AND ALTITUDES
C
C      SUBROUTINE OUTDIU (K,IDH,IEND,IS)
C      =====
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C
C      COMMON
C      -----
C
C      COMMON /CONC/ X1(0:99,0:33),X2(0:99,1:30)
C      COMMON /ISO/ Y(20,0:65,65)
C      COMMON /ZENITH/ ALPHA,BETA,TAU(0:99)
C
C      DECLARE
C      -----
C
C      REAL*8 Z(0:65,65)
C      CHARACTER*4 SUBST1(33),SUBST2(30),SUBST(65)
C      REAL*4 TIME(20),TIMX(0:99)
C      EQUIVALENCE (SUBST(1),SUBST1(1)),(SUBST(34),SUBST2(1))
C
C      DATA
C      ----
C
C      DATA SUBST1/
1'O2 ','O ODD','N ODD','H ODD','SOX ','HXS ','CLX ','CW ','DUM1',
2'DUM2','N2O ','NH3 ','NH4+','HNO3','H2 ','H2O ','WSSR','H2O2',
3'HSO4','COS ','CO ','CO2 ','CH4 ','C2H2','C2H6','C3H8','F11 ',
4'F12 ','CCL4','C3CL','CCL3','C2CL','HCL '/
C      DATA SUBST2/
1'O ','OS ','O3 ','N ','NO ','NO2 ','NO3 ','N2O5','HNO2',
2'HNO4','H ','OH ','HO2 ','SO ','SO2 ','HS ','H2S ','CL ',
3'ClO ','CL2 ','HOCL','CLNO','CHO ','CH3 ','CH2O','CH3O','CHO2',
4'DUM3','DUM4','DUM5'/
C      DATA TIME /12.00,14.00,15.00,16.00,17.15,17.45,17.58,18.00,18.15,
*19.00,21.00,24.00,3.00, 6.00, 6.02, 6.15, 6.45, 8.00, 9.00,10.00/
```

```
C      IANF=0
C
      GOTO (10,20,30),IS
10      DO 18 J=1,33
          DO 18 I=IANF,IEND,IDH
              Y(K,I,J)=X1(I,J)/X1(I,0)
18      CONTINUE
          DO 19 J=1,30
              DO 19 I=IANF,IEND,IDH
                  Y(K,I,J+33)=X2(I,J)/X1(I,0)
19      CONTINUE
          RETURN
C
20      IDHX=IDH*(((IEND-IANF)/IDH)/14+1)
          DO 25 J=1,63
              IF ((Y(20,1,J).EQ.0.).OR.(J.EQ.8)) GOTO 25
              DO 25 I=IANF,IEND,IDH
                  F0=1.D0
                  IF (Y(20,I,J).EQ.0.D0) GOTO 21
                  F0=Z(I,J)/Y(20,I,J)
21              DO 25 KX=1,20
                  ITIM=TIME(KX)
                  TX=ITIM+(TIME(KX)-ITIM)*100./60.
                  IF (KX.GT.12) TX=TX+24
                  Y(KX,I,J)=Y(KX,I,J)*(1.+(F0-1.)*(TX-10.)/24.)
25          CONTINUE
          WRITE (6,1004) ((I),I=IANF,IEND,IDHX)
          DO 28 KX=1,20
              DO 27 I=IANF,IEND,IDH
                  ITIM=TIME(KX)
                  TIM=ITIM+(TIME(KX)-ITIM)/.6
                  IF (TIME(KX).LT.6.) TIM=TIM*(2.-TAU(I))
                  IF ((TIME(KX).GE.6.).AND.(TIME(KX).LT.18.))
*                  TIM=(TIM-12.)*TAU(I)+12.
                  IF (TIME(KX).GE.18.) TIM=24.-(24-TIM)*(2.-TAU(I))
                  ITIM=TIM
                  TIMX(I)=ITIM+(TIM-ITIM)*.6
27          CONTINUE
          WRITE (6,1005) TIME(KX),(TIMX(I),I=IANF,IEND,IDHX)
28      CONTINUE
          DO 29 J0=1,63,2
              WRITE (6,1001)
              DO 29 J=J0,J0+1
                  WRITE (6,1002) SUBST(J),((I),I=IANF,IEND,IDHX)
                  DO 29 KX=1,20
                      WRITE (6,1003) TIME(KX),(Y(KX,I,J),I=IANF,IEND,IDHX)
29      CONTINUE
          IX=99
          WRITE (11) IX
          WRITE (11) ALPHA,BETA,TAU
          WRITE (11) Y
C
      RETURN
C
30      DO 38 J=1,33
          DO 38 I=IANF,IEND,IDH
              Z(I,J)=X1(I,J)/X1(I,0)
38      CONTINUE
          DO 39 J=1,30
              DO 39 I=IANF,IEND,IDH
                  Z(I,J+33)=X2(I,J)/X1(I,0)
39      CONTINUE
```

```
      RETURN
C
1001 FORMAT ('1',40X,'VOLUME MIXING RATIOS')
1002 FORMAT (/5X,A4/'0TIME ',I3,'KM',13I9/)
1003 FORMAT (F6.2,1P,14E9.2)
1004 FORMAT ('1',40X,'TIME'///'0TIME',I7,'KM',13I9/)
1005 FORMAT (F6.2,14F9.2)
      END
/*
```

```
//ICH301E5 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301E5,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C                      EEEE      5555
C                      E          5
C                      E--      5555
C                      E          5
C                      EEEE      555
```

```
C
C *****
C *                               *
C *  OUTPUT OF DIURNAL VARIATION PER MINUTE  *
C *                               *
C *****
```

```
C
C PURPOSE              : OUTPUT OF MIXING RATIOS OF ONE SPECIFIED COMPONENT
C                      : AT ABOUT EVERY MINUTE
C INPUT VIA CALL       : J : NUMBER OF SPECIFIED COMPONENT
C                      : LTIME: LOCAL TIME AT ALTITUDE I
C                      : IS:  SWITCH =1 : STORING OF DATA
C                      :                =2 : NORMALIZATION AND OUTPUT
C INPUT VIA COMMON     : C : CONCENTRATION PROFILES
C OUTPUT ON PRINTER:   TIME: LOCAL TIME
C                      : CNC : MIXING RATIO
C                      : X : FACTOR IN RELATION TO NOON VALUE
```

```
C      SUBROUTINE OUTMIN (J,LTIME,IS,IDH,IEND)
```

```
C      =====
C      REAL*8 LTIME (0:99),   C (0:99,0:63)
C      REAL*4 TIME (1440,14),  CNC (1440,14)
C      COMMON /CONC/ C
```

```
C      DATA K/0/
```

```
C      IANF=(IEND/IDH-13)*IDH
C      IF (IANF.LT.0) IANF=0
1  GOTO (10,20),IS
```

```
C      STORING
C      -----
```

```
10  K=K+1
    DO 19 IX=IANF,IEND,IDH
      I=(IX-IANF)/IDH+1
      CNC(K,I)=C(IX,J)/C(IX,0)
      IT=LTIME(IX)
      TIME(K,I)=IT+(LTIME(IX)-IT)*.6
19  CONTINUE
    IE=I
    IF ((LTIME(0).LE.12.01D0).AND.(LTIME(0).GT.11.D0)) K12=K
    RETURN
```

```
C      NORMALIZATION
C      -----
```

```
20  KEND=K
    DO 29 I=1,IE
      F=CNC(1,I)/(2.*CNC(KEND,I)-CNC(KEND-1,I))
      DO 29 K=1,KEND
        CNC(K,I)=CNC(K,I)*(F+(F-1.)/KEND*(K-KEND-1))
```

```
29 CONTINUE
C
C   OUTPUT
C   -----
      WRITE (6,1000) J,(I,I=IANF,IEND,IDH)
      DO 39 K=1,KEND
      WRITE (6,2000) (TIME(K,I),I=1,IE)
      WRITE (6,3000) (CNC(K,I),I=1,IE)
      WRITE (6,4000) ((CNC(K,I)/CNC(K12,I)),I=1,IE)
39 CONTINUE
C
C   FORMATS
C   -----
1000 FORMAT ('1',10X,'MIXING RATIOS AND NORMALIZATION FACTORS FOR COMPO
      *UND',I3/70X,'TIME : HOUR.MIN*10'//14I9,' KM'/)
2000 FORMAT (14F9.3,' TIME')
3000 FORMAT (1P,14E9.2,' MIXRAT')
4000 FORMAT (14F9.3,' FACTR'/)
5000 FORMAT (5I5,1P,5E12.3)
C
      RETURN
      END
/*
```

```
//ICH301F1 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301F1,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
C
C
C          FFFF      1
C          F      1 1
C          F      1
C          F      1
C
C
C *****
C *
C *      UNTERPROGRAMM: CALCULATION OF
C *      REACTION RATES
C *
C *****
C
C PURPOSE          : CALCULATION OF THE PRODUCTION RATES AND
C                   DESTRUCTION FREQUENCIES FOR EACH SINGLE
C                   ATMOSPHERIC COMPOUND AND FOR THE COMPOUND
C                   FAMILIES
C INPUT VIA CALL   : ISW: SWITCH      =0: OUTPUT FOR RATE VALUES
C                   =1: OUTPUT OF THE REACTION NUMBERS
C                   AND -SYMBOLS
C INPUT VIA COMMON : C: CONCENTRATION PROFILES
C                   RR: ACTUAL GASPHASE REACTION CONSTANTS
C                   RD: ACTUAL PHOTODISSOCIATION FREQUENCIES
C                   RN: ACTUAL WET REMOVAL FREQUENCIES
C                   NEP: REACTION SYMBOLS
C
C SUBROUTINE RATES (ISW)
C
C
C COMMON
C -----
C
C COMMON / ISWCH / IP(12)
C COMMON / CONC / C(0:99,0:63)
C COMMON / RATEAK / RR(200,0:99),RD(70,0:99),RN(20,0:99)
C COMMON / RATE / XR(200,0:99),XD(11,70,0:99),XRN(20,0:99),
1 AVK(200,2),NEP(300,6)
C
C DECLARE
C -----
C
C REAL *8 R(290,0:99),RR,RD,RN,XR,XD,XRN,AVK,C
C REAL *4 X(10,50)
C INTEGER *4 N(10,3),NS(70),NR(270),NSUM(10,7)
C CHARACTER*4 TEXT2(0:90)
C
C 1 FORMAT (3I10,5X,2I4,A2,3I4,10X,A4,' + ',A4,2X,' ---> ',
C *      2X,A4,' + ',A4,' + ',A4)
C 2 FORMAT ('1 DESTR.=1 SUBSTANCE REACTION',13X,'SYMBOL'/
C *      ' PROD.=2')
C 3 FORMAT ('0'/)
C
C DATA
C ----
C
C DATA NR /125*1,45*0,29*1,0,35*1,35*0/
C DATA NS/
```

```

1 34,35,00,01,00,00,36,37,38,39,40,00,11,41,00,00,12,44,45,46,
2 15,16,18,00,42,14,47,48,00,00,49,50,00,19,51,52,00,00,33,54,
3 00,00,00,53,21,22,56,58,57,59,60,00,00,00,00,23,24,25,00,26,
4 28,27,29,30,32,31,00,20,43,55/

```

```

DATA NSUM / 1, 2, 7, 0, 0, 0, 0, 0, 3, 2,
1          8, 9,10,11,14,25,69,70, 8, 3,
2          18,19,20,25,40,69, 0, 0, 6, 4,
3          35,36,40,44,70, 0, 0, 0, 5, 7,
4          27,28, 0, 0, 0, 0, 0, 0, 2, 5,
5          31,32, 0, 0, 0, 0, 0, 0, 2, 6,
6          47,48,49,50,51, 0, 0, 0, 5, 8/

```

C

```

DATA TEXT2 / '
1          'O','O1D','O1S','O2','O2D','O2S','O3'
2          'N','NO','NO2','NO3','N2','N2O','N2O5'
3          'NH','NH2','NH3','H','OH','HO2','H2'
4          'H2O','H2O2','HNO','HNO2','HNO3','SO','SO2'
5          'SO3','S2O','HS','H2S','HSO3','HSO4','CL'
6          'CLO','CLO2','CLO3','HCL','HOCL','HOC*','NOCL'
7          'NOC*','CL2','CO','CO2','CHO','CH2O','CH3'
8          'CH3O','C3O2','CHH*','COO*','CHN*','CH3*','CH4'
9          'C2H2','C2H6','59','C3H8','F12','F11','CCL4'
A          'CHCL','C2CL','CCL3','67','COS','HNO4','CLNO'
B          'HV','72','73','74','75','76','77'
C          'AIR','WSSR','NH4','OODD','NODD','HODD','CLX'
D          'SOX','HXS','CXHY','88','89','90' /

```

C

```

IF (ISW.EQ.1) THEN
  WRITE (6,2)
ELSE
  CALL GRSTRT (35,8)
END IF
DO 19 L=1,10
  DO 18 J=1,3
    N(L,J)=0
    X(L,J)=0.
18  CONTINUE
  DO 19 J=4,50
    X(L,J)=0.
19  CONTINUE

```

C

```

DO 29 I=0,99
  DO 27 J=271,290
    R(J,I)=RN(J-270,I)
27  CONTINUE
  DO 28 J=1,200
    R(J,I)=RR(J,I)
28  CONTINUE
  DO 29 J=201,270
    R(J,I)=RD(J-200,I)
29  CONTINUE
  L=1

```

C

```

DO 39 IT=1,2
  DO 38 IS=1,70
    ICC=NS(IS)
    IF (ICC.EQ.0) GOTO 38
    IF (ISW.EQ.1) WRITE (6,3)
    DO 37 IR=1,290
      IF (NR(IR).EQ.0) GOTO 37
      IDA=IT*IT
      IDE=IDA+IT
    DO 36 ID=IDA,IDE

```

```

      IF (NEP(IR,ID).NE.IS) GOTO 36
      IF (ISW.NE.1) GOTO 301
      IF (IR.GT.200) NEP(IR,2)=71
      WRITE (6,1) IT,IS,IR,
1      (NEP(IR,J),J=1,6),(TEXT2(NEP(IR,J)),J=1,2),
2      (TEXT2(NEP(IR,J)),J=4,6)
      GOTO 36
301  CONTINUE
      DO 35 J=1,3
      N(L,J)=NEP(IR,J)
35  CONTINUE
      DO 34 M=0,99,2
      IH=M/2+1
      IC=NEP(IR,1)
      IC=NS(IC)
      X(L,IH)=R(IR,M)*C(M,IC)
      IF (IR.GT.200) GOTO 302
      IC=NEP(IR,2)
      IF (IC.EQ.0) GOTO 302
      IC=NS(IC)
      IF (IC.NE.0) X(L,IH)=X(L,IH)*C(M,IC)
302  CONTINUE
      IC=NS(IS)
      IF ((IT.EQ.1).AND.(C(M,IC).NE.0.))
      *      X(L,IH)=X(L,IH)/C(M,IC)
34  CONTINUE
      L=L+1
      IF (L.LE.10) GOTO 36
      IS10=10
      CALL OUT (X,N,IS10,IS,IT,ICC)
      L=1
36  CONTINUE
37  CONTINUE
      L=L-1
      IF (L.NE.0) CALL OUT (X,N,L,IS,IT,ICC)
      L=1
38  CONTINUE
39  CONTINUE
C
C  FAMILIES
C  -----
C
400 DO 49 IT=1,2
      DO 48 IS=1,7
      ISS=IS+80
      ICC=NSUM(10,IS)
      ISE=NSUM( 9,IS)
      IF (ISW.EQ.1) WRITE (6,3)
      DO 47 IR=1,290
      IF (NR(IR).EQ.0) GOTO 47
      IY=0
      IDA=IT*IT
      IDE=IDA+IT
      DO 46 ID=IDA,IDE
      DO 45 IX=1,ISE
      IF (NEP(IR,ID).EQ.NSUM(IX,IS)) IY=IY+1
45  CONTINUE
46  CONTINUE
      IF (IY.EQ.0) GOTO 47
      IT1=3-IT
      IDA=IT1*IT1
      IDE=IDA+IT1
      DO 44 ID=IDA,IDE

```

```

DO 43 IX=1,ISE
  IF (NEP(IR,ID).EQ.NSUM(IX,IS)) IY=IY-1
43  CONTINUE
44  CONTINUE
  IF (IY.EQ.0) GOTO 47
  IF (ISW.NE.1) GOTO 401
  IF (IR.GT.200) NEP(IR,2)=71
  WRITE (6,1) IT,IS,IR,(NEP(IR,J),J=1,6),
1      (TEXT2(NEP(IR,J)),J=1,2),
2      (TEXT2(NEP(IR,J)),J=4,6)
  GOTO 47
401  CONTINUE
  DO 42 J=1,3
    N(L,J)=NEP(IR,J)
42  CONTINUE
  DO 41 M=0,99,2
    IH=M/2+1
    IC=NEP(IR,1)
    IC=NS(IC)
    X(L,IH)=R(IR,M)*C(M,IC)
    IF (IR.GT.200) GOTO 402
    IC=NEP(IR,2)
    IF (IC.EQ.0) GOTO 402
    IC=NS(IC)
    IF (IC.NE.0) X(L,IH)=X(L,IH)*C(M,IC)
402  CONTINUE
    IF ((IT.EQ.1).AND.(C(M,ICC).NE.0.))
      *      X(L,IH)=X(L,IH)/C(M,ICC)
41  CONTINUE
    L=L+1
    IF (L.LE.10) GOTO 47
    IS10=10
    CALL OUT (X,N,IS10,ISS,IT,ICC)
    L=1
47  CONTINUE
    L=L-1
    IF (L.NE.0) CALL OUT (X,N,L,ISS,IT,ICC)
    L=1
48  CONTINUE
49  CONTINUE
  IF (ISW.NE.1) CALL GREND
  RETURN
END

```

/*

```
//ICH301F2 JOB (324,035431),ROETH,CLASS=C,TIME=(00,09)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301F2,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//C.SYSIN DD *
```

```
C
C
C          FFFF      22
C          F      2  2
C          F      2
C          F      2222
```

```
C *****
C *
C *   UNTERPROGRAMM: OUTPUT OF REACTION RATES   *
C *
C *****
```

```
C PURPOSE          : OUTPUT OF ABSOLUTE OR RELATIVE REAKTION RATES AND
C                   FREQUENCIES ON PRINTER AND OF RELATIVE RATES ON
C                   PLOTTER
C INPUT VIA CALL   : X : RATES OR FREQUENCIES
C                   N : SYMBOL OF THE REACTION
C                   L : NUMBER OF REACTIONS TO BE PRINTED
C                   IS: INDEX OF THE APPROPRIATE COMPOUND
C                   IT: SWITCH   =1: DESTRUCTION FREQUENCIES
C                               =2: PRODUCTION RATES
C                   IC: INDEX OF THE OVERALL RATE
C INPUT VIA COMMON : P : OVERALL PRODUCTION RATES
C                   D : OVERALL DESTRUCTION FREQUENCIES
C                   IOUTRL: SWITCH =0: ABSOLUTE RATES PRINTED
C                               =1: RELATIVE RATES PRINTED
C                               =2: RELATIVE RATES PRINTED + PLOTTED
C OUTPUT ON PRINTER: X : RATES OR FREQUENCIES (ABSOLUTE OR RELATIVE)
C OUTPUT ON PLOTTER: X : RELATIVE RATES
```

```
      SUBROUTINE OUT (X,N,L,IS,IT,IC)
```

```
      COMMON
```

```
      COMMON /TERME/ P(0:99,2:63),D(0:99,2:63),TT(0:99,2:33)
      COMMON /ISWTCH/ IP(12)
```

```
      DECLARE
```

```
      REAL *8 P,D,TT
      REAL *4 X(10,50),R(52),H(52)
      INTEGER *4 N(10,3),IHV,MT
      CHARACTER*4 IHVX,MTX,TEXT1,TEXT(90)
      CHARACTER*3 HILF
      EQUIVALENCE (IHV,IHVX),(MT,MTX)
```

```
      DATA
```

```
      DATA      IHVX /'HV'/, MTX/'M '/, ISX /0/, IBILD /0/
      DATA      TEXT  /' O',' O1D',' O1S',' O2',' O2D',' O2S',' O3'
2              , ' N',' NO',' NO2',' NO3',' N2',' N2O',' N2O5'
3              , ' NH',' NH2',' NH3',' H',' OH',' HO2',' H2'
4              , ' H2O',' H2O2',' HNO',' HNO2',' HNO3',' SO',' SO2'
5              , ' SO3',' S2O',' HS',' H2S',' HSO3',' HSO4',' CL'
```

6	,	'CLO'	,	'CLO2'	,	'CLO3'	,	'HCL'	,	'HOCL'	,	'HOC*'	,	'NOCL'
7	,	'NOC*'	,	'CL2'	,	'CO'	,	'CO2'	,	'CHO'	,	'CH2O'	,	'CH3'
8	,	'CH3O'	,	'C3O2'	,	'CHH*'	,	'COO*'	,	'CHN*'	,	'CH3*'	,	'CH4'
9	,	'C2H2'	,	'C2H6'	,	'59'	,	'C3H8'	,	'F12'	,	'F11'	,	'CCL4'
A	,	'CHCL'	,	'C2CL'	,	'CCL3'	,	'67'	,	'COS'	,	'HNO4'	,	'CLNO'
B	,	'HV'	,	'72'	,	'73'	,	'74'	,	'75'	,	'76'	,	'77'
C	,	'AIR'	,	'WSSR'	,	'NH4'	,	'OODD'	,	'NODD'	,	'HODD'	,	'CLX'
D	,	'SOX'	,	'HXS'	,	'CXHY'	,	'88'	,	'89'	,	'90'	,	'/'

C
C
C
C

PRINT

MEND=41
IOUTRL=IP(9)
IF (ISX.NE.IS) WRITE (6,1300)
ISX=IS
IF (IT.EQ.1) WRITE (6,1000) TEXT(IS)
IF (IT.EQ.2) WRITE (6,1001) TEXT(IS)
WRITE (6,1100) ((N(I,J),J=1,3),I=1,L)
DO 19 M=1,MEND
IM=2*M-2
H(M)=IM
IF (IOUTRL.EQ.0) GOTO 18

C
C

RELATIVE RATES

DO 17 I=1,L
IF ((IT.EQ.1).AND.(D(IM,IC).NE.0.))
* X(I,M)=X(I,M)/D(IM,IC)
IF ((IT.EQ.2).AND.(P(IM,IC).NE.0.))
* X(I,M)=X(I,M)/P(IM,IC)
17 CONTINUE
18 CONTINUE
WRITE (6,1200) IM,(X(I,M),I=1,L)
19 CONTINUE
IF (IOUTRL.NE.2) RETURN

C
C
C
C

PLOTTEN

200 CONTINUE
R(MEND+1)=-4.
R(MEND+2)=1.
H(MEND+1)=0.
H(MEND+2)=10.
DO 29 I=1,L
XA=(I-1)*6.0-(I/6)*30.0+2.
YA=11.*(1-(I/6))+2.
XB=XA+4.
YB=YA+9.
CALL GRCHRC (.3,0.,16)
CALL GRSCLC (XA,YA,XB,YB)
CALL GRSCLV (-4.,0.,0.,90.)
CALL GRAXS (9,'X,Y,A,F=2',1,' ',1,' ')
DO 28 J=1,MEND
R(J)=ALOG10(AMAX1(1.E-4,X(I,J)))
28 CONTINUE
CALL GRLN (R,H,MEND)
XN=-3.5
YN=82.
ZAHL1=N(I,1)
ZAHL2=N(I,2)
CALL GRCHRC (.3,0.,16)
WRITE (HILF,'(F3.0)') ZAHL1

```
      CALL GRTXT (XN,YN,3,HILF)
      XN=XN+1.
      IF (N(I,2).NE.IHV) GOTO 201
      CALL GRTXT (XN,YN,2,'HV')
      GOTO 29
201   WRITE (HILF,'(F3.0)') ZAH2
      CALL GRTXT (XN,YN,3,HILF)
      IF (N(I,3).NE.MT) GOTO 29
      XN=XN+1.
      CALL GRTXT (XN,YN,1,'M')
29   CONTINUE
      CALL GRCHRC (.7,0.,24)
      TEXT1=TEXT(15)
      CALL GRTXT (1.,8.,4,TEXT1)
      IBILD=IBILD+1
      WRITE (6,1400) IBILD
      CALL GRNXTF
      RETURN
C
1000 FORMAT ('0',5X,A4,'-DESTRUCTION'//50X,'REACTION')
1001 FORMAT ('0',5X,A4,'-PRODUCTION'//50X,'REACTION')
1100 FORMAT (' ALT.',10(I7,I3,A2))
1200 FORMAT (' ',I5,1P,10E12.3)
1300 FORMAT ('1')
1400 FORMAT(/10X,'DATA PLOTTED ON FIG.',I5)
      END
```

/*

```
//ICH301F3 JOB (324,035431),ROETH,CLASS=C,TIME=(00,15)
/*PASSWORD MODEL
/*ROUTE PRINT MVS
//      EXEC CFORTV,DS='USER.ICH300.OBJECT',NAME=ICH301F3,
//      PARM.C='MAP,XREF,OPTIMIZE(2)',REGION=1024K
//SYSUT5 DD UNIT=TEMP,SPACE=(6400,200)
//C.SYSIN DD *
C
C
C          FFFF      333
C          F_        _3
C          F_        _3
C          F          333
C
C *****
C *
C *      SUBROUTINE FOR DIURNAL-AVERAGE COEFFICIENT
C *
C *****
C
C PURPOSE          : CALCULATION OF THE DIURNAL-AVERAGING
C                   COEFFICIENTS FOR REACTION RATES AND PHOTOLYSIS
C                   FREQUENCIES
C INPUT VIA CALL   : IDH   : ALTITUDINAL STEP
C                   IS     : SWITCH  =1: SUMMING UP
C                           =2: AVERAGING
C INPUT VIA COMMON : C     : CONCENTRATION PROFILES
C                   R,D    : RATES OF GASPHASE-REACTIONS AND OF PHOTOLYSIS
C                   NEP    : KEY FOR THE REACTION PARTNERS
C OUTPUT VIA COMMON: AVK   : AVERAGING COEFFICIENTS
C OUTPUT ON PRINTER: AVRAGE: AVERAGES FOR THE PHOTOLYSIS
C AND ON PUNCHER: AVK    : AVERAGING COEFFICIENTS FOR THE REACTION RATES
C
C      SUBROUTINE MEAN (IDH,IS)
C      =====
C
C      IMPLICIT REAL*8 (A-H,O-Z)
C
C      COMMON
C      -----
C
C      COMMON /CONC/ C(0:99,0:63)
C      COMMON /RATEAK/ R(200,0:99),D(70,0:99),RN(20,0:99)
C      COMMON /RATE/ XR(200,0:99),XD(11,70,0:99),XRN(20,0:99),AVK(200,2),
C      *          NEP(300,6)
C
C      DIMENSION
C      -----
C
C      DIMENSION CC(0:99,0:63),RR(200,0:99),DD(70,0:99),
C      *          AVRAGE(270,0:99)
C      INTEGER*4 NEP,NS(70)
C
C      DATA
C      ----
C
C      DATA NR/0/,CC/6400*0./,RR/20000*0./,DD/7000*0./
C      DATA NS/
1  34,35,00,01,00,00,36,37,38,39,40,00,11,41,00,00,12,44,45,46,
2  15,16,18,00,42,14,47,48,00,00,49,50,00,19,51,52,00,00,33,54,
3  00,00,00,53,21,22,56,58,57,59,60,00,00,00,00,23,24,25,00,26,
4  28,27,29,30,32,31,00,20,43,55/
C
C      IANF=0
```

```

      IEND=65
      JEND=40
C
C      SUMS
C      ----
C
10  IF (IS.NE.1) GOTO 200
      NR=NR+1
      DO 19 I=IANF,IEND,IDH
        DO 18 J=1,63
          CC(I,J)=CC(I,J)+C(I,J)
18    CONTINUE
        DO 17 J=1,200
          N1=NEP(J,1)
          N2=NEP(J,2)
          IF ((N1.EQ.0).OR.(N2.EQ.0)) GOTO 17
          N1=NS(N1)
          N2=NS(N2)
          RR(J,I)=RR(J,I)+C(I,N1)*C(I,N2)
17    CONTINUE
        DO 16 J=1,JEND
          N1=NEP(J+200,1)
          IF (N1.EQ.0) GOTO 16
          N1=NS(N1)
          DD(J,I)=DD(J,I)+D(J,I)*C(I,N1)
16    CONTINUE
19    CONTINUE
      RETURN
C
C      MEANS
C      =====
C
C      GASPHASE REACTIONS
C      -----
C
200 IF (IS.NE.2) RETURN
      ISTD=(1+4/IDH)*IDH
      WRITE (6,2000) NR,((IX),IX=0,IEND,ISTD)
      DO 29 J=1,200
        DO 28 I=IANF,IEND,IDH
          AVRAGE(J,I)=1.
          N1=NEP(J,1)
          N2=NEP(J,2)
          IF ((N1.EQ.0).OR.(N2.EQ.0)) GOTO 28
          N1=NS(N1)
          N2=NS(N2)
          IF ((CC(I,N1).LT.1.E-20).OR.(CC(I,N2).LT.1.E-20)) GOTO 28
          AVRAGE(J,I)=RR(J,I)/CC(I,N1)*NR/CC(I,N2)
28    CONTINUE
        WRITE (6,2001) J,(AVRAGE(J,I),I=IANF,IEND,ISTD)
29    CONTINUE
C
C      COEFFICIENTS OF GASPHASE REACTIONS
C      -----
C
      DO 49 J=1,200
        S1=0.
        S2=0.
        S3=0.
        S4=0.
        S5=0.
        DO 48 I=IANF,IEND,IDH
          Y=AVRAGE(J,I)

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```

      S1=S1+1.
      S2=S2+I
      S3=S3+I*I
      S4=S4+Y
      S5=S5+I*Y
48  CONTINUE
      AVK(J,1)=1.
      AVK(J,2)=0.
      DIV=S2*S2-S1*S3
      IF (DIV.EQ.0.) GOTO 49
      AVK(J,1)=(S2*S5-S4*S3)/DIV
      AVK(J,2)=(S2*S4-S1*S5)/DIV
49  CONTINUE
      WRITE (6,4000)
      DO 59 J=1,200,3
        J1=J+1
        J2=J+2
        WRITE (6,5000) J,AVK(J,1),AVK(J,2),J1,AVK(J1,1),AVK(J1,2),
1      J2,AVK(J2,1),AVK(J2,2)
        WRITE (9,5000) J,AVK(J,1),AVK(J,2),J1,AVK(J1,1),AVK(J1,2),
1      J2,AVK(J2,1),AVK(J2,2)
59  CONTINUE
C
C  PHOTOLYSIS
C  -----
C
      WRITE (6,3000) ((IX),IX=0,IEND,ISTP)
      DO 39 J=201,240
        DO 38 I=IANF,IEND,IDH
          AVRG(J,I)=1.
          N1=NEP(J,1)
          IF (N1.EQ.0) GOTO 38
          N1=NS(N1)
          IF ((CC(I,N1).LT.1.E-20).OR.(D(J-200,I).LT.1.E-40)) GOTO 38
          AVRG(J,I)=DD(J-200,I)/CC(I,N1)/D(J-200,I)
38  CONTINUE
        WRITE (9,2002) J-200
        WRITE (9,3001) (AVRG(J,I),I=IANF,IEND,ISTP)
        WRITE (6,2001) J-200,(AVRG(J,I),I=IANF,IEND,ISTP)
39  CONTINUE
      AVRG=1.DO
      WRITE (9,3002) (AVRG,I=IANF,IEND,ISTP)
      WRITE (6,3002)
      WRITE (6,1000)
      RETURN
C
C  FORMAT
C  -----
C
1000 FORMAT (/////'O AVERAGING COEFFICIENTS PUNCHED')
2000 FORMAT ('1 AVERAGES',5X,'FROM',I3,' DATA'/' REACT',15I8)
2001 FORMAT (I6,15F8.4)
2002 FORMAT (I4)
3000 FORMAT ('1 PHOTODISSOCIATION AVERAGES'/' REACT',15I8)
3001 FORMAT (1X,1P,7E10.2)
3002 FORMAT ('0 ACHTUNG! NO-PHOTOLYSE AUF 1 AENDERN'/(1X,1P,7E10.2))
4000 FORMAT ('1 AVERAGING COEFFICIENTS',10X,'AV.COEFF.=A+B*Z'
*      /3(' NR',5X,'A',9X,'B',4X))
5000 FORMAT (1X,3(I4,1P,2E10.2))
      END
/*

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