

Review and Improvement of Methods for Estimating Rates of Photolysis in Photochemical Models

Volume II: User's Guide for TUVAQM Radiative Transfer and Photolysis Module

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1 Introduction

This manual describes the TUV AQM module for calculating solar actinic flux and photolysis rates within air quality models (or on a standalone basis), based on the Tropospheric Ultraviolet Visible (TUV) radiation transfer program (version 3.9) by Dr. Sasha Madronich of the National Center for Atmospheric Research (NCAR). TUV AQM is designed to be callable from another program such as an Air Quality Model (AQM). The package includes library routines, test programs, UNIX installing scripts, and supporting data. The object of TUV AQM is to compute the solar actinic flux at a given location and time given specific atmospheric conditions. Photolysis reaction rate coefficients can be computed by TUV AQM providing the cross sections and quantum yields are available. The relationship between solar actinic flux and photolysis reaction rates, as well as the definition of these quantities is discussed in section 2. Section 2 also summarizes the theoretical background that supports the radiation transfer model.

The radiation transfer calculations depend on a large number of parameters that describe the atmospheric optical and other properties. Most of these parameters are given reasonable default values in the library routines, however the user can (and sometime must) provide some parameter values for describing specific situations. The parameter values can be set via input files whose syntax is described in section 5 and 6. The library routines can either be used within an Air Quality Model or for simulating a standalone radiation transfer model.

When TUV AQM is used within a standalone radiation transfer program (see section 4), the situation is unique for each simulation, corresponding to the conditions at a given time and location. Thus, the parameters values are fixed for the given time and location, and their values can be set with the input file described in section 5.

When TUV AQM is used within an air quality model (see section 3), a range of conditions can occur depending on the modeling domain cell (location) and modeling time. Some parameters may remain constant throughout the whole domain and modeling episode, and some others may vary from cell-to-cell and time-to-time. The approach chosen is to select a reduced number of important parameters that are given values that depend on time and space and let the other parameters apply to the whole AQM simulation. The parameters that depend on time and space can be set with the input file described in section 6. Parameters that do not vary spatially or temporally are set in the same manner as for a standalone simulation (file described in section 5).

TUV AQM has been installed in the following air quality models: Urban Airshed Model (UAM-IV), Urban Airshed Model with flexible chemical mechanism (UAM-FCM), and the SARMAP Air Quality Model (SAQM). For use of TUV AQM with these air quality models, the user should

review sections 3 and 4, and the execution instructions in sections 5 and 6. If the user wishes to install TUVAQM in another air quality model or install a standalone version of the program, a more detailed knowledge of the module structure is needed, and the user should also review installation instructions (section 7) and the code description (section 8).

2 Theoretical background

This section summarizes the key elements for establishing the mathematical expressions used to represent the radiative transfer in TUVAQM. A more detailed description is given in section II of Volume I of this report.

2.1 Actinic flux and photolysis rate coefficients

Radiation transfer models are used to obtain theoretical estimations of quantities that depend on the radiation flux. Examples of such quantities include, but are not limited to, coefficients determining the speed of chemical reactions (photolysis) induced by solar radiation in the atmosphere, solar radiation flux, radiation effects on living species, and heating of the earth by solar radiation. Two quantities of importance for this purpose are the actinic flux and the irradiance. Both measure the amount of light that crosses a unit surface area per unit of time, and per unit interval of wavelength. The actinic flux is the spherically-integrated light intensity that is appropriate for calculating photolysis reaction rate coefficients (see Madronich, 1987). The irradiance refers to a flux across a horizontal plane; sunlight intensity is commonly measured and reported in terms of irradiance. The actinic flux F and irradiance I as a function of frequency $\nu = hc/\lambda$ are defined by:

$$\begin{aligned} F(\nu) &\equiv \int d\phi \int d\theta u_\nu(\theta, \phi) \sin \theta \\ I(\nu) &\equiv \int d\phi \int d\theta u_\nu(\theta, \phi) \cos \theta \sin \theta \end{aligned} \quad (1)$$

where $u_\nu(\theta, \phi)$ is the spectral radiance (sometime also called radiation specific intensity or, simply, intensity) associated with a specific zenith angle θ and azimuth angle ϕ .

In the context of air quality modeling, radiation transfer models are of interest for computing photolysis rate coefficients J . The rate of chemical species photolysis via a given reaction X is found by multiplying J_X with the concentration of the species undergoing the photolysis. The photolysis rate coefficient J_X is evaluated by integrating over wavelengths using the relationship

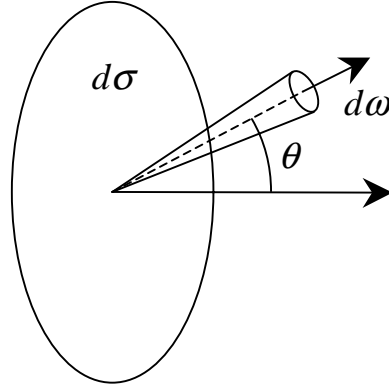
$$J_X = \int_0^\infty \sigma_X(\lambda) \phi_X(\lambda) F(\lambda) d\lambda \quad (2)$$

where $\sigma_X(\lambda)$ is the absorption cross section (cm^2), $\phi_X(\lambda)$ is the quantum yield, and $F(\lambda)$ is the actinic flux ($\text{photons cm}^{-2} \text{s}^{-1} \text{nm}^{-1}$). For a specific molecule reacting in the troposphere, the lower

limit of integration is frequently set $\lambda = 290$ nm and the higher limit is the longest wavelength where the photochemical reaction occurs (the reaction threshold). Most photolysis reactions of interest for air quality occur in the wavelength region $\lambda = 290$ to 420 nm (i.e., the near UV).

2.2 Radiation transfer general equation

The object of the radiation transfer package described in this manual is to determine how the radiance propagates through the atmosphere. Most radiation transfer models are based on theoretical developments attributed to Chandrasekhar (1960). Chandrasekhar defines the radiance u_ν at frequency ν by its relationship to “the amount of radiant energy dE_ν , in a frequency interval $(\nu, \nu + d\nu)$, which is transported across an element of area $d\sigma$ and in directions confined to an element of solid angle $d\omega$ during a time dt ”:



$$dE_\nu = u_\nu \cos \theta \, d\nu \, d\sigma \, d\omega \, dt \quad (3)$$

When the radiation transfer occurs in an atmosphere composed of parallel horizontal layers, the radiance transfer equation can be expressed as (see Liou, 1973 or Stamnes *et al.*, 1988):

$$\begin{aligned} \mu \frac{du_\nu(\tau_\nu, \mu, \phi)}{d\tau_\nu} = & u_\nu(\tau_\nu, \mu, \phi) \\ & - \frac{\omega_\nu(\tau_\nu)}{4\pi} \int_0^{2\pi} d\phi' \int d\mu' P_\nu(\tau_\nu, \mu, \phi, \mu', \phi') u_\nu(\tau_\nu, \mu', \phi') \\ & - Q_\nu(\tau_\nu, \mu, \phi) \end{aligned} \quad (4)$$

Eq. (4) describes the radiance transfer in the direction defined by μ the cosine of the zenith angle and ϕ the azimuth angle at the altitude z corresponding to the optical depth τ_ν defined by:

$$\tau_\nu = \int_z^\infty k_\nu \rho \, dz \quad (5)$$

where k_ν is the extinction coefficient and ρ the density. The first term of the right-hand side of Eq. 4 is a loss term proportional to the radiance. The remainder of the right-hand side is a source term split into a scattering source term and another term, Q_ν , covering all other sources. The scattering source term expresses the amount of radiance that is scattered from the direction (μ', ϕ') into the direction (μ, ϕ) . $P_\nu(\tau_\nu, \mu, \phi, \mu', \phi')$ is the phase function, and $\omega_\nu(\tau_\nu)$ is the single scattering albedo. While a term for thermal emission in local thermodynamic equilibrium is

sometime included in Q_ν , only the contribution from the direct solar beam will be considered here. In this case,

$$Q_\nu = \frac{\omega_\nu(\tau_\nu)}{4} F_{0\nu} P_\nu(\tau_\nu, \mu, \phi, -\mu_0, \phi_0) \exp\left(-\frac{\tau_\nu}{\mu_0}\right) \quad (6)$$

where πF_0 is the incident solar flux coming from the direction (μ_0, ϕ_0) . When there is no explicit radiance transfer from one frequency to another (the thermal emission term can be viewed as an implicit transfer of radiance), the frequency index ν can be dropped for simplicity without loss of generality.

Analytical solutions of Eq. (4) can only be found in simplified cases, and numerical methods are often used. The main difficulty comes from the integration over the whole solid angle in the scattering source term. Most methods for finding analytical or numerical solutions to Eq. (4) have common features that were devised by Chandrasekhar. The first step common to almost all methods is to simplify the integration over the azimuth angle in Eq. 4 by expanding the radiance in a Fourier cosine series:

$$u(\tau, \mu, \phi) = \sum_{m=0}^{2N-1} u^m(\tau, \mu) \cos m(\phi_0 - \phi), \quad (7)$$

and the phase function in a sum of Legendre polynomials that, by using the addition theorem for spherical harmonics, is transformed to:

$$P(\tau, \mu, \phi, \mu', \phi') = \sum_{m=0}^{2N-1} (2 - \delta_{0,m}) \cos m(\phi' - \phi) \sum_{l=m}^{2N-1} (2l+1) g_l^m(\tau) P_l^m(\mu) P_l^m(\mu') \quad (8)$$

where g_l^m are sets of constants that are determined using the orthogonal property of Legendre polynomials. A set of $2N$ decoupled equations (one for each Fourier component) is obtained:

$$\begin{aligned} \mu \frac{du^m(\tau, \mu)}{d\tau} &= u^m(\tau, \mu) \\ &- \frac{\omega(\tau)}{2} \sum_{l=m}^{2N-1} (2l+1) g_l^m(\tau) P_l^m(\mu) \int_{-1}^{+1} d\mu' P_l^m(\mu') u^m(\tau, \mu') \\ &- \frac{\omega(\tau)}{4} F_0 \exp\left(-\frac{\tau}{\mu_0}\right) (2 - \delta_{0,m}) \sum_{l=m}^{2N-1} (-1)^{l+m} (2l+1) g_l^m(\tau) P_l^m(\mu) P_l^m(\mu_0) \end{aligned} \quad (9)$$

2.3 Two-stream methods

In two-stream methods (see Meador and Weaver, 1980), it is assumed that only two streams of radiation (i.e., two directions) exist. Both streams are vertical, one going downward, and the

other upward. In such a case, the solution is symmetric with respect of the azimuth angle, and only the equation for $m = 0$ in Eq. (9) should be retained. Defining $p(\tau, \mu, \mu')$ as:

$$p(\tau, \mu, \mu') = \omega(\tau) \sum_{l=0}^{2N-1} (2l+1) g_l^0(\tau) P_l^0(\mu) P_l^0(\mu'), \quad (10)$$

the following transfer equation is obtained (the superscript index $m=0$ is dropped for simplicity):

$$\begin{aligned} \mu \frac{du(\tau, \mu)}{d\tau} &= u(\tau, \mu) \\ &\quad - \frac{1}{2} \int_{-1}^{+1} d\mu' p(\tau, \mu, \mu') u(\tau, \mu') \\ &\quad - \frac{1}{4} F_0 \exp\left(-\frac{\tau}{\mu_0}\right) p(\tau, \mu, -\mu_0) \end{aligned} \quad (11)$$

The streams are defined as the following hemispheric integrals:

$$u^\pm(\tau) = \int_0^1 u^\pm(\tau, \pm\mu) \mu d\mu, \quad (12)$$

and the quantity β_0 is defined as:

$$\beta_0(\tau) = \frac{1}{2\omega(\tau)} \int_0^1 p(\tau, \mu, -\mu_0) d\mu. \quad (13)$$

Because the phase function is normalized as $\int_{-1}^1 p(\tau, \mu, \mu') d\mu' = 2\omega(\tau)$, then

$$\beta_0(\tau) = 1 - \frac{1}{2\omega(\tau)} \int_0^1 p(\tau, -\mu, -\mu_0) d\mu. \quad (14)$$

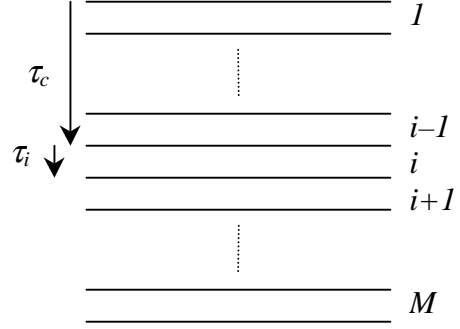
Thus, after integrating Eq. (11) from 0 to 1 along μ in one case and $-\mu$ in the other, the following pair of equation is obtained:

$$\begin{aligned} \frac{du^+(\tau)}{d\tau} &= \int_0^1 u(\tau, \mu) d\mu \\ &\quad - \frac{1}{2} \int_0^1 d\mu \int_{-1}^{+1} d\mu' p(\tau, \mu, \mu') u(\tau, \mu') - \frac{1}{2} F_0 \omega(\tau) \beta_0(\tau) \exp\left(-\frac{\tau}{\mu_0}\right) \\ \frac{du^-(\tau)}{d\tau} &= - \int_0^1 u(\tau, -\mu) d\mu \\ &\quad + \frac{1}{2} \int_0^1 d\mu \int_{-1}^{+1} d\mu' p(\tau, -\mu, \mu') u(\tau, \mu') + \frac{1}{2} F_0 \omega(\tau) (1 - \beta_0(\tau)) \exp\left(-\frac{\tau}{\mu_0}\right) \end{aligned} \quad (15)$$

The two-stream methods approximate $u(\tau, \mu)$ so that it is related to $u^\pm(\tau)$ to obtain the following general form for the transfer equation:

$$\begin{aligned}
\frac{du^+(\tau)}{d\tau} &= \gamma_1 u^+(\tau) - \gamma_2 u^-(\tau) - F_0 \omega(\tau) \gamma_3 \exp\left(-\frac{\tau}{\mu_0}\right) \\
\frac{du^-(\tau)}{d\tau} &= \gamma_2 u^+(\tau) - \gamma_1 u^-(\tau) + F_0 \omega(\tau) \gamma_4 \exp\left(-\frac{\tau}{\mu_0}\right)
\end{aligned} \tag{16}$$

The parameters γ_1 , γ_2 , γ_3 , and γ_4 , depend on the assumed functional form $p(\tau, \mu, \mu')$. For the most commonly chosen functional forms, γ_1 , γ_2 , γ_3 , and γ_4 are simple functions of the single scattering albedo $\omega(\tau)$, the asymmetry parameter $g(\tau)$ and μ_0 . Consequently, the γ parameters depend on τ . In order to solve the coupled Eqs. (16), the atmosphere is divided in thin horizontal layers where the parameters are assumed constant¹. Within a layer, Toon *et al.* (1989) have shown that the general solution to the coupled Eqs. (16) is:



$$\begin{aligned}
u_i^+(\tau) &= k_{1i} \exp(\lambda_i \tau) - \Gamma_i k_{2i} \exp(-\lambda_i \tau) + C_i^+(\tau) \\
u_i^-(\tau) &= \Gamma_i k_{1i} \exp(\lambda_i \tau) - k_{2i} \exp(-\lambda_i \tau) + C_i^-(\tau)
\end{aligned} \tag{17}$$

where the index i stands for the layer number, k_1 and k_2 depend on the boundary conditions, and by assuming a layer of optical depth τ_i and cumulative optical depth τ_c for the layers above,

$$\begin{aligned}
\lambda_i &= \sqrt{\gamma_{1i}^2 - \gamma_{2i}^2} \\
\Gamma_i &= \frac{\gamma_{2i}}{\gamma_{1i} + \lambda_i} \\
C_i^+(\tau) &= \frac{\omega_i \pi F_0 [(\gamma_{1i} - 1/\mu_0) \gamma_{3i} + \gamma_{4i} \gamma_{2i}] \exp[-(\tau_c + \tau)/\mu_0]}{\lambda_i^2 - 1/\mu_0} \\
C_i^-(\tau) &= \frac{\omega_i \pi F_0 [(\gamma_{1i} + 1/\mu_0) \gamma_{4i} + \gamma_{2i} \gamma_{3i}] \exp[-(\tau_c + \tau)/\mu_0]}{\lambda_i^2 - 1/\mu_0}
\end{aligned} \tag{18}$$

First, Toon *et al.* scaled the terms so that none of them includes a positive τ -dependent exponent (terms with such positive exponents can lead to numerical instabilities):

¹ When deriving the solution, the layers are assumed to be planar. Corrections are made afterward to take into account the atmosphere sphericity. Such corrections are only important for large solar zenith angle.

$$\begin{aligned}
u_i^+(\tau) &= Y_{1i}(\exp[-\lambda_i(\tau_i - \tau)] + \Gamma_i \exp[-\lambda_i \tau]) \\
&+ Y_{2i}(\exp[-\lambda_i(\tau_i - \tau)] - \Gamma_i \exp[-\lambda_i \tau]) + C_i^+(\tau) \\
u_i^-(\tau) &= Y_{1i}(\Gamma_i \exp[-\lambda_i(\tau_i - \tau)] + \exp[-\lambda_i \tau]) \\
&+ Y_{2i}(\Gamma_i \exp[-\lambda_i(\tau_i - \tau)] - \exp[-\lambda_i \tau]) + C_i^-(\tau)
\end{aligned} \tag{19}$$

where $\tau < \tau_i$, since τ_i is the total optical depth of the layer, and

$$\begin{aligned}
Y_{1i} &= \frac{1}{2}(k_{1i} \exp(\lambda_i \tau_i) + k_{2i}) \\
Y_{2i} &= \frac{1}{2}(k_{1i} \exp(\lambda_i \tau_i) - k_{2i})
\end{aligned} \tag{20}$$

Then, an iterative solution scheme is devised from one layer to the other by requesting:

$$\begin{aligned}
u_i^+(\tau = \tau_i) &= u_{i+1}^+(\tau = 0) \\
u_i^-(\tau = \tau_i) &= u_{i+1}^-(\tau = 0) \\
u_1^-(\tau = 0) &= u_{d0}^- \\
u_M^+(\tau = \tau_M) &= R_{\text{sfc}}(u_M^-(\tau = \tau_M) + \mu_0 \pi F_0 \exp[-(\tau_c + \tau_M)/\mu_0])
\end{aligned} \tag{21}$$

where u_{d0}^- is a diffuse downward flux at the top of the atmosphere (usually set to 0), M is the total number of layers, and R_{sfc} is the ground surface reflectivity (albedo).

After rearranging the terms, Toon *et al.* found a set of $2M$ equations that compose a tridiagonal matrix of the form:

$$\begin{aligned}
A_j Y_{j-1} + B_j Y_j + D_j Y_{j+1} &= E_j \\
Y_j &= Y_{1i} \quad j = 2n - 1 \quad (\text{odd}) \\
Y_j &= Y_{2i} \quad j = 2n \quad (\text{even})
\end{aligned} \tag{22}$$

that is solved using a standard tridiagonal solution method. Once a solution is found for the expressions Y_{1i} and Y_{2i} , the solution for the upward and downward flux can be derived via Eq. (19), and the actinic flux defined in Eq. 1 can be computed with (Toon *et al.* 1989):

$$F_i = \frac{u_i^+ + u_i^-}{\mu_1}, \tag{23}$$

where μ_1 is a parameter that depends on the chosen two-stream approximation.

The type of two-stream approximation used defines the γ parameters. Meador and Weaver (1980) and Toon *et al.* (1989) gave the value of these parameters for different type of two-stream methods. The method used in TUV AQM is the delta-scaled Eddington approximation. Code for other approximations is also included but inactivated (commented out). To use one of these other

approximations, the user needs to make code changes in SUBROUTINE PS2STR in file rad_tr.f (see section 8).

2.4 Other methods

One version of the original Tropospheric Ultraviolet Visible (TUV) radiation transfer program uses the discrete ordinate method. This method and other related methods are more complex than two-stream approximations, and allow a more precise description of the angular dependence of the radiance. They rely on applying a Gaussian quadrature rule to integrate over the zenith angle following Eq. (9). (For details, see Chandrasekhar, 1960, Liou, 1973 or Stamnes *et al.*, 1988.) The integral over μ' is replaced by a discrete sum over quadrature zenith angle using Gauss quadrature. For each of the $2N$ equations for the Fourier component a set of $2n$ coupled equations should be solved (one for each of the quadrature zenith angles):

$$\begin{aligned} \mu_i \frac{du^m(\tau, \mu_i)}{d\tau} = & u^m(\tau, \mu_i) \\ & - \frac{\omega(\tau)}{2} \sum_{l=m}^{2N-1} (2l+1) g_l^m(\tau) P_l^m(\mu_i) \sum_{\substack{j=-n \\ j \neq 0}}^n a_j P_l^m(\mu_j) u^m(\tau, \mu_j) \\ & - \frac{\omega(\tau)}{4\pi} I_0 \exp\left(-\frac{\tau}{\mu_0}\right) (2 - \delta_{0,m}) \times \\ & \sum_{l=m}^{2N-1} (-1)^{l+m} (2l+1) g_l^m(\tau) P_l^m(\mu_i) P_l^m(\mu_0) \quad i = \pm 1, \dots, \pm n \end{aligned} \quad (24)$$

The discrete-ordinate method and the other related methods allow an arbitrarily precise description of the radiance angular dependence, according to the number of terms considered. At the lowest order ($m = 0$, and $n = 1$), they reduce to a two-stream method. When good precision in the angular description is desired, the dimensionality of the equation system is large. There are $M \times 2n \times 2N$ equations, where M is the number of atmospheric horizontal layers, $2n$ is the number of Gaussian quadrature zenith angles, and $2N$ is the number of Fourier azimuth components².

3 Using the library within an AQM

TUVAQM can be used in the framework on an air quality model (AQM) for determining rate coefficients for the photolysis reactions. For using TUVAQM, the main AQM program needs only to call a single generic routine (subroutine tuvaqm). This routine can be called in an initialization mode (hopefully once in the AQM program execution) or in the normal execution

² The number of Fourier components is usually restricted by assumptions over the functional form of the phase function.

mode (every time a photolysis reaction rate coefficient evaluation is needed in the AQM). Many factors influence radiation transfer in the atmosphere. These factors are parameters that are inputs to the program and their values can be set via input files. The following parameters must be defined in TUV AQM:

- 1) General parameters such as date, time, time zone, longitude, latitude, and zenith angle.
- 2) Elevation grid, i.e., the vertical column structure the program uses for the computations.
- 3) Wavelength grid, i.e., the wavelength bins the program uses for the computations.
- 4) Air pressure.
- 5) Absorption and scattering by aerosols.
- 6) Absorption and scattering by clouds.
- 7) Ground albedo.
- 8) Air temperature.
- 9) Absorption by ozone.
- 10) Absorption by SO₂.
- 11) Absorption by NO₂.
- 12) Extraterrestrial solar flux.

Reasonable default values are provided for these parameters, and the user can change the values using a general input file read at initialization time (see section 5). Values set this way will be used for the whole AQM simulation. However, multiple situations can occur depending on the modeling domain cell (location) and modeling time. Thus, some parameters may apply throughout the whole domain and modeling period, while some others should be allowed to vary from cell to cell and time to time. Unfortunately, data that can be used to specify these parameters are usually scarce, and the spatial and temporal resolution is often poor. The strategy chosen in the current implementation is to select a reduced number of parameters that can vary within the AQM simulation domain and episode. These parameters are:

- 1) zenith angle,
- 2) elevation grid,
- 3) ground albedo,
- 4) total ozone column,
- 5) total aerosol optical depth,
- 6) aerosol single scattering albedo, and
- 7) aerosol asymmetry factor.

The user *must* specify the temporal and spatial dependence for these values. First, the user must divide the modeling domain into regions and the modeling episode into time intervals such that the atmospheric properties can be considered as constant within a given region and time interval. Then the user needs to specify the parameter values for each region and time interval using the input file described in section 6.

For each region and time interval, a set of complete radiation transfer calculations will be performed for conditions representative of the region and time interval. For all AQM spatial cells within a region, and time steps within an interval, the photolysis reaction rate coefficients will be computed by interpolation from the full radiation transfer calculations.

4 Using the library with a standalone program

TUVAQM consists of two classes of routines: generic routines that perform groups of tasks and basic routines that perform a single task. Typically, the generic routines use the basic routines to perform groups of tasks such as initialization, or a full radiation transfer calculation. The generic routines can be used to create a standalone radiation transfer simulation program. Examples of such programs are provided, and the instructions for installing them are given in section 7. These examples include one program for performing a single simulation and another for repeated simulations with a reduced set of parameters (up to five) varied in a systematic way for sensitivity studies.

The example programs read an input file for setting the simulation conditions (the parameters listed in section 3), compute one or more simulations and, depending on the version (see section 7), save the results of the simulations. The following section describes the syntax of the input file.

The library routines can also be used for creating a new radiation transfer simulation program. The section 8 gives an overview of the test program as well as the generic and basic libraries.

5 General card and command description

The general card and command input file allows changing the default values of the parameters describing the radiation transfer situation being simulated. Technically, this means setting values for code variables or variable arrays. In simple cases, a *card* key word is followed by a list of values. In more complex cases, when sets of values need to be changed in a coherent way, a *command* key word is followed by other key words and values.

5.1 Card description and syntax

A card is a segment of the input file (possibly extending over several lines) that starts with a card key word in the *first four columns* of the first line and is followed by a list of values ending when the next key word is encountered. Each card is used to set the value(s) for one parameter assigned in the computer code to one variable or variable array. Consequently each card key word is linked to one code variable of a given type and length. The types can be logical, integer, real, double precision, and character strings. Character strings are restricted to strings with a multiple of four characters. The length is equal to the number of elements of the corresponding variable array.

Example

```
TEMD 288.150 281.651 275.154
```

The card key word is TEMD (linked to the internal variable array TMPDEF) that is used to define the atmospheric temperature profile. In the example the three lowest points of the temperature elevation grid are given the values 288.150, 281.651 and 275.154 K.

The list of values consists of values separated by one or more blank characters or tabulation characters. In order to facilitate setting values for an array, *locators* and *repetitors* can be used. A locator is an integer index followed by an equal sign (=) immediately preceding a value. The locator indicates that the following value is for the given index in the variable array corresponding to the card key word. A repetitor is an integer number n followed by a star sign (*) immediately preceding a value. The repetitor indicates that the given value is for n indices of the variable array, starting from the current index.

Example

```
TEMD 3*290.0 6*280 25=273.15 4*2.73E+02 15=278 275.
```

Indices 1, 2 and 3 of variable TMPDEF have the value 290 K, indices 4 to 9 have the value 280 K, index 25 has the value 273.15 K, indices 26 to 29 have the value 273 K, index 15 has the value 278 K and index 16 has the value 275 K. As shown in the example, indices can be skipped, locators can be given in any order, and indices increase monotonically starting from the last given locator or 1 if no previous locator is given.

In order to increase the readability of the input file, comment lines starting with an exclamation mark can be included at any time,

Example

```
!
!   Number of elevation grid levels
!
NBZG 46
!
!   Defines elevation grid levels (kilometers above sea level)
!
!           height   top of cell
!           elevation
!   ground elevation:           260 m
!   cell   1           50 m     310 m
!   cell   2           100 m    410 m
!   cell   3           300 m    710 m
!   cell   4          1290 m    2000 m
!   cell   5          2000 m    4000 m
!   cell   6          3000 m    7000 m
!   cell   7          5000 m   12000 m
!   cell   8-46         1000 m to 50000 m
!
! Cell 1-7
ZGRD 0.26 0.31 0.41 0.71 2.00 4.00 7.00
! Cell 8-46
      12.00 13.00 14.00 15.00 16.00 17.00 18.00 19.00 20.00
      21.00 22.00 23.00 24.00 25.00 26.00 27.00 28.00 29.00 30.00
      31.00 32.00 33.00 34.00 35.00 36.00 37.00 38.00 39.00 40.00
      41.00 42.00 43.00 44.00 45.00 46.00 47.00 48.00 49.00 50.00
```

NBZG and ZGRD are linked to variables describing the program general elevation grid. The number of elevations in the grid is set to 46, and the corresponding elevations are given. Comments are included to explain the grid structure.

The format for the values is the following:

- Logical values are ".TRUE." or ".FALSE.".
- Numbers can be given in integer, floating point or exponential notation.
- Character strings should be single quoted.

Cards can be omitted and values can be skipped within a card. In such a case, the default value is used. Cards can be given in any order, and can appear more than once. In case the same index of the same card is defined more than once, the last defined value is used. A description of all the recognized card key words with the corresponding variable, type and dimension, as well as the default values and description of the use of the variable in TUVAQM is given below.

5.1.1 Card list

5.1.1.1 General parameters:

The following variables are used to define general conditions of the simulation such as time and location for the simulations. It is possible to request TUVAQM to determine the solar zenith angle or to define the zenith angle as an input parameter. When TUVAQM determines the zenith angle, the location and time are important. When the zenith angle is an input parameter, time and location are ignored.

- Card key word: LIST

Code variable: LISCRD Type: LOGICAL Dimension: 1

Description:

Logical switch for printing user's card value. When this card is set to .TRUE. , the card values are printed after the input file is read.

Default: .FALSE.

- Card key word: DATE

Code variable: IDATE Type: INTEGER Dimension: 1

Description:

Decimal date (YYMMDD). This variable is used when one wants TUVAQM to compute the zenith angle. If the zenith angle is provided, this variable has no influence on the library routines.

Default: 970701

- Card key word: LATI

Code variable: ALAT Type: REAL Dimension: 1

Description:

Latitude (degree). This variable is used when one wants TUVAQM to compute the zenith angle. If the zenith angle is provided, this variable has no influence on the library routines. Latitude is between 0 and 90° for the Northern Hemisphere, and 0 and -90° for the Southern Hemisphere.

Default: 34.0

- Card key word: LONG

Code variable: ALONG Type: REAL Dimension: 1

Description:

Longitude (degree). This variable is used when one wants TUV AQM to compute the zenith angle. If the zenith angle is provided, this variable has no influence on the library routines. The longitude is between 0 and 180° for longitudes east of Greenwich Meridian, and between 0 and -180° for longitudes west of Greenwich Meridian.

Default: -117.3

- Card key word: UTSH

Code variable: UT0 Type: REAL Dimension: 1

Description:

Universal time shift (hours), i.e., the time difference between GMT and the local time. This variable is used when one wants TUV AQM to compute the zenith angle. If the zenith angle is provided, this variable has no influence on the library routines. This variable is used for conversion between the local time zone and the universal time. Regions west of Greenwich Meridian need a positive value, and region east of Greenwich Meridian a negative positive one. UTSH is 8 for Pacific Standard Time, and 7 for Pacific Daylight Time.

Default: 8.5

- Card key word: LTIM

Code variable: LUTIME Type: LOGICAL Dimension: 1

Description:

Logical switch for zenith angle computation. When this card is set to .TRUE., the zenith angle is computed at the desired time steps, given the location and date.

Default: .FALSE.

- Card key word: NSTO

Code variable: NBSTOP Type: INTEGER Dimension: 1

Description:

Number of times or zenith angles at which radiation transfer computations are requested.

Default: 13

- Card key word: SPNT

Code variable: S_PNTS Type: REAL

Dimension: MAX_ST = 100

Description:

Times or zenith angles at which radiation transfer computations are requested.

Default: 0.0, 5.0, 10.0, 20.0, 30.0, 40.0, 50.0, 60.0, 70.0,
 80.0, 85.0, 88.0, 90.0, 87*0.0

5.1.1.2 Wavelength and elevation general grid choice:

The following variables are used in SUBROUTINE TUV_RD. They define the segmentation in wavelength and elevation that TUV AQM uses to compute solar irradiance. Many inputs are given on their own wavelength or elevation grid. These grids do not coincide with the general wavelength or elevation grid. Library routines interpolate the input grids on the general grid.

- Card key word: CHWL

Code variable: MOPT_GW Type: INTEGER

Dimension: 1

Description:

Flag designating which wavelength grid is used. The options are:

- 1 = equal spacing
- 2 = Isaksen's grid
- 3 = Combined Kockarts/Isaksen's grid
- 4 = User defined

Default: 2 (Note: option 4 requires recoding)

- Card key word: NBZG

Code variable: NZ Type: INTEGER

Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) in the general elevation grid. In case NZ = 0, a regular elevation grid with 51 levels starting at 0 km and ending at 50 km is chosen.

Default: 0 (i.e., 51 levels.)

- Card key word: ZGRD

Code variable: Z Type: REAL Dimension: KZ = 101

Description:

Elevation cell boundaries in the general elevation grid. In case NZ = 0 (see NBZG), a regular elevation grid with 51 levels starting at 0 km and ending at 50 km is chosen. If the elevation grid is defined by the user, it must be in strictly ascending order.

Default: KZ * 0 i.e. 51 levels {0,1,2,3,...,50} (see NBZG)

5.1.1.3 Air pressure (air density) definition:

The following variables are used in SUBROUTINE SETAIR. The air density is given for layers of the atmosphere where the density is assumed to be constant.

- Card key word: APTI

Code variable: APRTIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the air pressure elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'air density: USSA, 1976' '

- Card key word: APRN

Code variable: APRNEW Type: REAL Dimension: 1

Description:

Sea level air pressure. An air density elevation profile can be defined (see below). In general, the sea level air pressure is defined by summing the air density elevation profile. If a sea level pressure is given, the air density profile is adjusted (scaled) such that the sea level air pressure is equal to APRNEW. When APRNEW is less than zero, the sea level pressure is determined by summing the air density profile.

Default: -999.0 i.e., sea level pressure defined by air density elevation profile.

- Card key word: APNZ

Code variable: NBAPRZ Type: INTEGER

Dimension: 1

Description:

Number of air pressure elevation profile grid cell limits.

Default: 121

- Card key word: APZG

Code variable: ZG_APR Type: REAL

Dimension: KZGAPR = 151

Description:

Air density elevation profile grid, i.e., levels at which the air density is given. The air density elevation grid must be in a strictly ascending order. The elevation grid is given in kilometer.

Default: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
 11, 12, 13, 14, 15, 16, 17, 18, 19, 20,
 21, 22, 23, 24, 25, 26, 27, 28, 29, 30,
 31, 32, 33, 34, 35, 36, 37, 38, 39, 40,
 41, 42, 43, 44, 45, 46, 47, 48, 49, 50,
 51, 52, 53, 54, 55, 56, 57, 58, 59, 60,
 61, 62, 63, 64, 65, 66, 67, 68, 69, 70,
 71, 72, 73, 74, 75, 76, 77, 78, 79, 80,
 81, 82, 83, 84, 85, 86, 87, 88, 89, 90,
 91, 92, 93, 94, 95, 96, 97, 98, 99, 100,
 101, 102, 103, 104, 105, 106, 107, 108, 109, 110,
 111, 112, 113, 114, 115, 116, 117, 118, 119, 120,
 30*-1

- Card key word: APRD

Code variable: APRDEF Type: REAL

Dimension: KZGAPR = 151

Description:

Air density elevation profile, i.e., air density at altitude levels of elevation grid. Default values are annual means from US Standard Atmosphere, 1976, for 45N (See NOAA, 1976). Values are number density (cm^{-3}).

Default: 2.55E+19, 2.31E+19, 2.09E+19, 1.89E+19, 1.70E+19,
 1.53E+19, 1.37E+19, 1.23E+19, 1.09E+19, 9.71E+18,
 8.60E+18, 7.59E+18, 6.49E+18, 5.54E+18, 4.74E+18,

```

4.05E+18, 3.46E+18, 2.96E+18, 2.53E+18, 2.16E+18,
1.85E+18, 1.57E+18, 1.34E+18, 1.14E+18, 9.76E+17,
8.33E+17, 7.12E+17, 6.09E+17, 5.21E+17, 4.47E+17,
3.83E+17, 3.28E+17, 2.82E+17, 2.41E+17, 2.06E+17,
1.76E+17, 1.51E+17, 1.30E+17, 1.12E+17, 9.62E+16,
8.31E+16, 7.19E+16, 6.23E+16, 5.40E+16, 4.70E+16,
4.09E+16, 3.56E+16, 3.11E+16, 2.74E+16, 2.42E+16,
2.14E+16, 1.89E+16, 1.68E+16, 1.49E+16, 1.33E+16,
1.18E+16, 1.05E+16, 9.30E+15, 8.24E+15, 7.29E+15,
6.44E+15, 5.68E+15, 5.00E+15, 4.40E+15, 3.87E+15,
3.39E+15, 2.97E+15, 2.60E+15, 2.27E+15, 1.98E+15,
1.72E+15, 1.50E+15, 1.30E+15, 1.12E+15, 9.64E+14,
8.30E+14, 7.13E+14, 6.12E+14, 5.25E+14, 4.49E+14,
3.84E+14, 3.27E+14, 2.79E+14, 2.37E+14, 2.02E+14,
1.71E+14, 1.44E+14, 1.21E+14, 1.01E+14, 8.50E+13,
7.12E+13, 5.96E+13, 4.99E+13, 4.18E+13, 3.49E+13,
2.92E+13, 2.44E+13, 2.04E+13, 1.70E+13, 1.42E+13,
1.19E+13, 9.99E+12, 8.40E+12, 7.07E+12, 5.96E+12,
5.02E+12, 4.24E+12, 3.58E+12, 3.02E+12, 2.55E+12,
2.14E+12, 1.80E+12, 1.52E+12, 1.30E+12, 1.11E+12,
9.68E+11, 8.43E+11, 7.38E+11, 6.50E+11, 5.75E+11,
5.10E+11, 30*0

```

- Card key word: APRH

Code variable: APRHSC Type: REAL

Dimension: 1

Description:

Air density scale height.

Default: 8.05E+05

5.1.1.4 Scaling and interpolation

Several of the atmospheric optical parameters described below are interpolated and can be scaled. The interpolation is done because the parameters are each given on an elevation profile grid that is specific to the parameter considered. For performing the radiative transfer calculations, TUV AQM interpolates the results given on the specific grids to its general grid. When a specific grid is larger than the general grid (e.g., a parameter is given from the sea level to the

top of the atmosphere, and the general grid starts from a ground elevation above sea level), part of the specific grid is chopped off to fit into the general grid. The scaling is done to change an elevation profile so that its sum corresponds to a given value. For example, a default aerosol optical depth elevation profile is given. It is possible to give a total aerosol optical depth, and request that the aerosol optical depth of each elevation grid cell will be scaled so that the total aerosol optical depth (the sum over the elevation cells) will correspond to the given value. In such a case, it is important to know if the scaling is done before or after the interpolation. In case a part of the specific elevation grid is chopped off, scaling done before interpolation will consider the full sum, while scaling done after interpolation will consider the partial sum fitting into the general grid. Both options can be valid. If a quantity is usually given for the whole atmosphere (e.g., sea-level air pressure or ozone total column), it makes sense to scale before interpolation. If a quantity is usually given at a given site considering only the portion of the atmosphere above the given site, it makes sense to scale after interpolation. For each of the following quantity that can be scaled, a note indicates whether the scaling is done before or after the interpolation. Changing this order can be accomplished only by changing the computer code (see section 8).

5.1.1.5 Aerosol definition:

The following variables are used in SUBROUTINE SETAER. The aerosol profile is given for atmospheric elevation layers in which the aerosol density and other properties are assumed constant. The aerosol optical depth per kilometer at 340 nm is given for each layer. For computing the aerosol optical depth at other wavelengths, TUV AQM assumes the optical depth to be inversely proportional to the first power of the wavelength:

$$\tau(\lambda) = \frac{\lambda_{340}}{\lambda} \tau(\lambda_{340})$$

where τ is the optical depth and λ the wavelength.

- Card key word: AETI

Code variable: AERTIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the aerosol elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'Aerosols: Elterman (1968) '

- Card key word: AERF

Code variable: AEROSL Type: LOGICAL Dimension: 1

Description:

Logical switch for using aerosol. If the switch is set to . FALSE ., the aerosol total optical depth is automatically set to zero.

Default: . FALSE .

- Card key word: AODN

Code variable: AODNEW Type: REAL Dimension: 1

Description:

Total vertical aerosol optical depth. An aerosol optical depth elevation profile can be defined by specifying the aerosol optical depth of each aerosol elevation profile cell (see below). In general, the total vertical aerosol optical depth is defined by summing the aerosol optical depths over the elevation profile. If a total vertical aerosol optical depth is given, the aerosol elevation cell optical depths are adjusted (scaled) such that the total vertical aerosol optical depth is equal to AODNEW.

When AODNEW is less than zero, the total vertical aerosol optical depth is determined by summing the aerosol optical depths over the elevation profile.

AODNEW is the total optical depth for light at wavelength = 340 nm.

Note: Because the aerosol elevation grid is interpolated on the general elevation grid, it matters whether the scaling is performed before or after the interpolation (see section 5.1.1.4). The scaling is done on the full aerosol profile before interpolation, and not on the aerosol profile on the general grid.

Default: -999.0 i.e., total aerosol optical depth defined by its elevation profile.

- Card key word: AENZ

Code variable: NBAERZ Type: INTEGER Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the aerosol elevation profile grid.

Default: 51

- Card key word: AEZG

Code variable: ZG_AER Type: REAL

Dimension: KZGAER = 101

Description:

Aerosol elevation profile grid, i.e., levels at which the aerosol optical depth and other properties are given. The aerosol elevation grid must be in a strictly ascending order. The elevation grid is given in kilometers.

Default: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
11, 12, 13, 14, 15, 16, 17, 18, 19, 20,
21, 22, 23, 24, 25, 26, 27, 28, 29, 30,
31, 32, 33, 34, 35, 36, 37, 38, 39, 40,
41, 42, 43, 44, 45, 46, 47, 48, 49, 50,
50*-1

- Card key word: AODD

Code variable: AODDEF Type: REAL

Dimension: KZGAER = 101

Description:

Aerosol optical depth elevation profile, i.e., aerosol optical depth per kilometer at altitude levels of the aerosol elevation grid. Values are from Elterman (1968).

These are vertical optical depths per km, in 1 km intervals from 0 km to 50 km, for light at wavelength = 340 nm. The total aerosol optical depth at 340 nm, assuming a linear behavior between elevation points, is 0.38.

Default: 2.40E-01, 1.06E-01, 4.56E-02, 1.91E-02, 1.01E-02,
7.63E-03, 5.38E-03, 5.00E-03, 5.15E-03, 4.94E-03,
4.82E-03, 4.51E-03, 4.74E-03, 4.37E-03, 4.28E-03,
4.03E-03, 3.83E-03, 3.78E-03, 3.88E-03, 3.08E-03,
2.26E-03, 1.64E-03, 1.23E-03, 9.45E-04, 7.49E-04,
6.30E-04, 5.50E-04, 4.21E-04, 3.22E-04, 2.48E-04,
1.90E-04, 1.45E-04, 1.11E-04, 8.51E-05, 6.52E-05,
5.00E-05, 3.83E-05, 2.93E-05, 2.25E-05, 1.72E-05,
1.32E-05, 1.01E-05, 7.72E-06, 5.91E-06, 4.53E-06,
3.46E-06, 2.66E-06, 2.04E-06, 1.56E-06, 1.19E-06,
9.14E-07, 50*0

- Card key word: AOMD
Code variable: AOMDEF Type: REAL Dimension: KZGAER = 101
Description:
Aerosol single scattering albedo elevation profile, i.e., aerosol single scattering albedo at altitude levels of the aerosol elevation grid.
Default: KZGAER * 0.99
- Card key word: AGDE
Code variable: AG_DEF Type: REAL Dimension: KZGAER = 101
Description:
Aerosol asymmetry factor elevation profile, i.e., aerosol asymmetry factor at altitude levels of the aerosol elevation grid.
Default: KZGAER * 0.61

5.1.1.6 Cloud definition:

The following variables are used in SUBROUTINE SETCLD. Since TUVAQM considers only one spatial dimension (elevation), partial cloud coverage and the effects of cloud edges cannot be represented in this model. It is possible to include some cloud layers that are treated in a way similar to the aerosols. Four cloud layers are defined; however, the default is set to simulate a clear sky situation (all cloud layers have zero optical depths).

- Card key word: CLTI
Code variable: CLDTIT Type: CHARACTER*32 Dimension: 1
Description:
Title for the cloud elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.
Default: 'Default zero cloud optical depth'
- Card key word: CLNZ
Code variable: NBCLDZ Type: INTEGER Dimension: 1
Description:
Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the cloud elevation profile grid.
Default: 4

- Card key word: CLZG
Code variable: ZG_CLD Type: REAL Dimension: KZGCLD = 21
Description:
Cloud elevation profile grid, i.e., levels at which the cloud optical depth and other properties are given. The cloud elevation grid must be in a strictly ascending order. The elevation grid is given in kilometers.
Default: 5, 7, 9, 11, 17*0
- Card key word: CODD
Code variable: CODDEF Type: REAL Dimension: KZGCLD = 21
Description:
Cloud optical depth elevation profile, i.e., cloud optical depth per kilometer at altitude levels of the cloud elevation grid. All optical depths are set to zero for simulating a clear-sky situation.
Default: KZGCLD * 0
- Card key word: COMD
Code variable: COMDEF Type: REAL Dimension: KZGCLD = 21
Description:
Cloud single scattering albedo elevation profile, i.e., cloud single scattering albedo in cells of the cloud elevation grid.
Default: 0.9999, 0.5, 0.9999, 18*0
- Card key word: CGDE
Code variable: CG_DEF Type: REAL Dimension: KZGCLD = 21
Description:
Cloud asymmetry factor elevation profile, i.e., cloud asymmetry factor in cells of the cloud elevation grid.
Default: 0.85, 0.5, 0.85, 18*0

5.1.1.7 Ground albedo definition:

The following variables are used in SUBROUTINE SETALB. The ground albedo can be defined on wavelength bins. The default is to define a ground albedo valid at all wavelengths.

- Card key word: ALBT
Code variable: ALBTIT Type: CHARACTER*32 Dimension: 1
Description:
Title for the ground albedo definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.
Default: 'Wavelength-independent albedo '
- Card key word: ALNW
Code variable: NBALBW Type: INTEGER Dimension: 1
Description:
Number of ground albedo wavelength profile grid bins.
Default: 1
- Card key word: ALWG
Code variable: WG_ALB Type: REAL Dimension: KWGALB = 100
Description:
Ground albedo wavelength profile grid, i.e., wavelengths at which the ground albedo is given. The ground albedo wavelength grid must be in a strictly ascending order. The wavelength grid is given in nanometers.
Default: 0.0, 1000.0, 98*-1
- Card key word: ALBD
Code variable: ALBDEF Type: REAL Dimension: KWGALB = 100
Description:
Ground albedo wavelength profile, i.e., ground albedo at boundaries of wavelength grid bins. The default is a wavelength-independent ground albedo defined on one bin that covers the whole wavelength range.
Default: 0.10, 0.10, 98*0

5.1.1.8 Atmospheric temperature definition:

The following variables are used in SUBROUTINE SETTMP. The air density is given for layers of the atmosphere where the density is assumed to be constant.

- Card key word: TMTI

Code variable: TMPTIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the atmospheric temperature elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'air temperature: USSA, 1976 '

- Card key word: TMNZ

Code variable: NBTMPZ Type: INTEGER Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the atmospheric temperature elevation profile.

Default: 121

- Card key word: TMZG

Code variable: ZG_TMP Type: REAL Dimension: KZGTMP = 201

Description:

Atmospheric temperature elevation profile grid, i.e., levels at which the atmospheric temperature is given. The atmospheric temperature elevation grid must be in a strictly ascending order. The elevation grid is given in kilometers.

Default: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10,
 11, 12, 13, 14, 15, 16, 17, 18, 19, 20,
 21, 22, 23, 24, 25, 26, 27, 28, 29, 30,
 31, 32, 33, 34, 35, 36, 37, 38, 39, 40,
 41, 42, 43, 44, 45, 46, 47, 48, 49, 50,
 51, 52, 53, 54, 55, 56, 57, 58, 59, 60,
 61, 62, 63, 64, 65, 66, 67, 68, 69, 70,
 71, 72, 73, 74, 75, 76, 77, 78, 79, 80,
 81, 82, 83, 84, 85, 86, 87, 88, 89, 90,
 91, 92, 93, 94, 95, 96, 97, 98, 99, 100,
 101, 102, 103, 104, 105, 106, 107, 108, 109, 110,
 111, 112, 113, 114, 115, 116, 117, 118, 119, 120,
 80*-1

- Card key word: TEMD

Code variable: TMPDEF Type: REAL

Dimension: KZGTMP = 201

Description:

Atmospheric temperature elevation profile, i.e., atmospheric temperature at altitude levels of elevation grid. Values are annual means from US Standard Atmosphere, 1976, for 45N (See NOAA, 1976). Temperatures are in Kelvin (K).

Default: 288.150 , 281.651 , 275.154 , 268.659 , 262.166 , 255.676 ,
 249.187 , 242.700 , 236.215 , 229.733 , 223.252 , 216.774 ,
 216.650 , 216.650 , 216.650 , 216.650 , 216.650 , 216.650 ,
 216.650 , 216.650 , 216.650 , 217.581 , 218.574 , 219.567 ,
 220.560 , 221.552 , 222.544 , 223.536 , 224.527 , 225.518 ,
 226.509 , 227.500 , 228.490 , 230.973 , 233.743 , 236.513 ,
 239.282 , 242.050 , 244.818 , 247.584 , 250.350 , 253.114 ,
 255.878 , 258.641 , 261.403 , 264.164 , 266.925 , 269.684 ,
 270.650 , 270.650 , 270.650 , 270.650 , 269.031 , 266.277 ,
 263.524 , 260.771 , 258.019 , 255.268 , 252.518 , 249.769 ,
 247.021 , 244.274 , 241.524 , 238.781 , 236.036 , 233.292 ,
 230.549 , 227.807 , 225.065 , 222.325 , 219.585 , 216.846 ,
 214.263 , 212.308 , 210.353 , 208.399 , 206.446 , 204.493 ,
 202.541 , 200.590 , 198.639 , 196.688 , 194.739 , 192.790 ,
 190.841 , 188.893 , 186.87 , 186.87 , 186.87 , 186.87 ,
 186.87 , 186.87 , 186.96 , 187.25 , 187.74 , 188.42 ,
 189.31 , 190.40 , 191.72 , 193.28 , 195.08 , 197.16 ,
 199.53 , 202.23 , 205.31 , 208.84 , 212.89 , 217.63 ,
 223.29 , 230.33 , 240.00 , 252.00 , 264.00 , 276.00 ,
 288.00 , 300.00 , 312.00 , 324.00 , 336.00 , 348.00 ,
 360.00 , 80*0

5.1.1.9 Ozone elevation profile definition:

The following variables are used in SUBROUTINE SETOZO. The ozone density is given for layers of the atmosphere where the density is assumed to be constant.

- Card key word: O3_T

Code variable: OZOTIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the ozone elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'ozone profile: USSA, 1976 '

- Card key word: O3_N

Code variable: OZONEW Type: REAL Dimension: 1

Description:

Overhead ozone total column in Dobson Units (DU). One DU is the thickness, measured in units of hundredths of a millimeter, that the ozone column would occupy at standard temperature and pressure. $1 \text{ DU} \approx 2.69 \cdot 10^{16} \text{ molecules cm}^{-2}$. An ozone density elevation profile can be defined (see below). For every cell of the ozone elevation profile, the ozone density is converted to a “partial ozone column”, and the default ozone total column is defined by summing all the ozone partial columns. If a new ozone column is given, the ozone density profile is adjusted (scaled) such that the ozone total column is equal to OZONEW. When OZONEW is less than zero, the ozone column is determined by summing the ozone partial columns.

Note: Because the ozone elevation grid is interpolated on the general elevation grid, it matters whether the scaling is performed before or after the interpolation (see section 5.1.1.4). The scaling is done on the profile on the general grid after interpolation, and not on the original ozone profile before interpolation.

Default: -999.0 i.e., ozone column defined by ozone density elevation profile.

- Card key word: O3NZ

Code variable: NBOZOZ Type: INTEGER Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the ozone elevation profile.

Default: 39

- Card key word: O3ZG

Code variable: ZG_OZO Type: REAL

Dimension: KZGOZO = 51

Description:

Ozone density elevation profile grid, i.e., levels at which the ozone density is given. The ozone density elevation grid must be in a strictly ascending order. The elevation grid is given in kilometers.

Default: 0, 1, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20,
22, 24, 26, 28, 30, 32, 34, 36, 38, 40,
42, 44, 46, 48, 50, 52, 54, 56, 58, 60,
62, 64, 66, 68, 70, 72, 74, 12*-1

- Card key word: O3_D

Code variable: OZODEF Type: REAL

Dimension: KZGOZO = 51

Description:

Ozone density elevation profile, i.e., ozone density at altitude levels of elevation grid. Values from 2 to 74 km are annual means from US Standard Atmosphere, 1976, for 45N (See NOAA, 1976) and values at 0 and 1 km are computed assuming a surface mixing ratio of 40 ppb and standard atmosphere. Values are number density ($n_{O_3} \text{ cm}^{-3}$). The total ozone column, assuming a linear behavior between elevation points, is 349.82 DU.

Default: 1.02E+12, 9.2E+11, 6.8E+11, 5.8E+11, 5.7E+11,
6.5E+11, 1.13E+12, 2.02E+12, 2.35E+12, 2.95E+12,
4.04E+12, 4.77E+12, 4.86E+12, 4.54E+12, 4.03E+12,
3.24E+12, 2.52E+12, 2.03E+12, 1.58E+12, 1.22E+12,
8.73E+11, 6.07E+11, 3.98E+11, 2.74E+11, 1.69E+11,
1.03E+11, 6.64E+10, 3.84E+10, 2.55E+10, 1.61E+10,
1.12E+10, 7.33E+09, 4.81E+09, 3.17E+09, 1.72E+09,
7.5E+08, 5.4E+08, 2.2E+08, 1.7E+08, 12*0

- Card key word: O3_H

Code variable: OZOHSC Type: REAL

Dimension: 1

Description:

Ozone density scale height.

Default: 4.50E+05

5.1.1.10 SO₂ molecule elevation profile definition:

The following variables are used in SUBROUTINE SETSO2. The SO₂ molecular density is given for layers of the atmosphere where the density is assumed to be constant. Note: the treatment of SO₂ and NO₂ molecules is identical.

- Card key word: SO2T

Code variable: SO2TIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the SO₂ molecule elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'Default SO2 1 ppb < 1km, 0 above'

- Card key word: SO2N

Code variable: SO2NEW Type: REAL Dimension: 1

Description:

Overhead SO₂ total column (in molec cm⁻²). An SO₂ molecular density elevation profile can be defined (see below). For every cell of the SO₂ elevation profile, the SO₂ molecular density is converted to a “partial SO₂ column”, and the default SO₂ total column is obtained by summing all the SO₂ partial columns. If a new SO₂ total column is given, the SO₂ molecular density profile is adjusted (scaled) such that the SO₂ total column is equal to SO2NEW. When SO2NEW is less than zero, the SO₂ column is determined by summing the SO₂ partial columns.

Note: Because the SO₂ elevation grid is interpolated on the general elevation grid, it matters whether the scaling is performed before or after the interpolation (see section 5.1.1.4). The scaling is done on the profile on the general grid after interpolation, and not on the original SO₂ molecule profile before interpolation.

Default: -999.0 i.e., SO₂ column defined by SO₂ density elevation profile.

- Card key word: SO2Z

Code variable: NBSO2Z Type: INTEGER Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the SO₂ elevation profile.

Default: 3

- Card key word: SO2G

Code variable: ZG_SO2 Type: REAL Dimension: KZGSO2 = 11

Description:

SO₂ molecular density elevation profile grid, i.e., levels at which the SO₂ molecular density is given. The SO₂ molecular density elevation grid must be in a strictly ascending order. The elevation grid is given in kilometer.

Default: 0, 1, 1.000001, 8*0
- Card key word: SO2D

Code variable: SO2DEF Type: REAL Dimension: KZGSO2 = 11

Description:

SO₂ molecular density elevation profile, i.e., SO₂ molecular density at altitude levels of elevation grid. Values are number density ($n_{\text{SO}_2} \text{ cm}^{-3}$). The default values correspond to 1 ppb of SO₂ molecule in the lowest kilometer of the atmosphere and zero above. Given the standard atmosphere, 1 ppb is equivalent to $2.69 \cdot 10^{10} \text{ cm}^{-3}$.

Default: 2.69E10, 2.69E10, 0, 8*0
- Card key word: SO2H

Code variable: SO2HSC Type: REAL Dimension: 1

Description:

SO₂ molecular density scale height.

Default: 4.50E+05

5.1.1.11 NO₂ molecule elevation profile definition:

The following variables are used in SUBROUTINE SETNO2. The NO₂ molecular density is given for layers of the atmosphere where the density is assumed to be constant. Note: the treatment of SO₂ and NO₂ molecules is identical.

- Card key word: NO2T

Code variable: NO2TIT Type: CHARACTER*32 Dimension: 1

Description:

Title for the NO₂ molecule elevation profile definition. This variable does not influence the radiation transfer simulation and is only used when input values are printed out.

Default: 'Default NO2 1 ppb < 1km, 0 above'

- Card key word: NO2N

Code variable: NO2NEW Type: REAL

Dimension: 1

Description:

Overhead NO₂ total column (in molec cm⁻²). An NO₂ molecular density elevation profile can be defined (see below). For every cell of the NO₂ elevation profile, the NO₂ molecular density is converted to a “partial NO₂ column”, and the default NO₂ total column is obtained by summing all the NO₂ partial columns. If a new NO₂ total column is given, the NO₂ molecular density profile is adjusted (scaled) such that the NO₂ total column is equal to NO2NEW. When NO2NEW is less than zero, the NO₂ column is determined by summing the NO₂ partial columns.

Note: Because the NO₂ elevation grid is interpolated on the general elevation grid, it matters whether the scaling is performed before or after the interpolation (see section 5.1.1.4). The scaling is done on the profile on the general grid after interpolation, and not on the original NO₂ molecule profile before interpolation.

Default: -999.0 i.e., NO₂ column defined by NO₂ density elevation profile.

- Card key word: NO2Z

Code variable: NBNO2Z Type: INTEGER

Dimension: 1

Description:

Number of elevation cell boundaries (i.e., the number of elevation cells plus 1) for the NO₂ elevation profile.

Default: 3

- Card key word: NO2G

Code variable: ZG_NO2 Type: REAL

Dimension: KZGNO2 = 11

Description:

NO₂ molecular density elevation profile grid, i.e., levels at which the NO₂ molecular density is given. The NO₂ molecular density elevation grid must be in a strictly ascending order. The elevation grid is given in kilometer.

Default: 0, 1, 1.000001, 8*0

- Card key word: NO2D
Code variable: NO2DEF Type: REAL Dimension: KZGNO2 = 11
Description:
NO₂ molecular density elevation profile, i.e., NO₂ molecular density at altitude levels of elevation grid. Values are number density ($n_{\text{NO}_2} \text{ cm}^{-3}$). The default values correspond to 1 ppb of NO₂ molecule in the lowest kilometer of the atmosphere and zero above. Given the standard atmosphere, 1 ppb is equivalent to $2.69 \cdot 10^{10} \text{ cm}^{-3}$.
Default: 2.69E10, 2.69E10, 0, 8*0
- Card key word: NO2H
Code variable: NO2HSC Type: REAL Dimension: 1
Description:
NO₂ molecular density scale height.
Default: 4.50E+05

5.2 Command description and syntax

A command is a line of the input file starting with a command key word in the *four first columns* of the line. While the card syntax is the same for every card, the command syntax depends on the command. In general, the command consists of the command key word followed by values and possibly other key words.

While cards are used to set code variable values with one to one correspondence between card key words and code variables, commands are used to request TUV AQM to perform some actions such as reading files, for example.

Example

```
!
! Scales aerosols total optical depth by +/- 20%
SCAN AODD(:51) 4 0.80 1.20 REL
```

The command key word is SCAN that is used to indicate which parameter is varied for sensitivity analysis. SCAN is followed by a card key word such as AODD. Other values and key words follow.

Commands can be omitted. When commands are not given, default actions will be executed. The SCAN command has an influence only when using executable s_tuv... for sensitivity analysis. When using other programs or an AQM (see section 7), the SCAN command has no effect.

5.2.1 Command list

5.2.1.1 End-of-file command

- Command key word: END

Command syntax: END

Description:

When the END command is encountered, TUV AQM initialization routine stops to read the general cards and commands input file. Whatever is after the END command is not read.

5.2.1.2 Sensitivity analysis SCAN command

A test program is provided with TUV AQM for sensitivity analysis (see section 7). Sensitivity analysis is performed by varying parameters in a given number of steps between given limits. Several parameters can be varied simultaneously (up to five). When more than one parameter is varied, the sensitivity analysis program systematically computes a radiation transfer simulation for all combination of the varying parameters. The parameters that can be varied are the parameters that can be set with the card key words. In case an AQM program or a test program other than the sensitivity analysis program is used, the SCAN command has no effect.

- Command key word: SCAN

Command syntax: SCAN Card # of steps Limits Key words

Description:

SCAN is used for repeating radiation transfer simulation with one or more parameter varied in a systematic way. The parameter to be varied is defined by the card key word given after the SCAN command. The card key word refers to one of the key words described in section 5.1. (Note: Only a limited set of the variables linked to the card key words can be varied with SCAN. These are of type INTEGER, REAL or DOUBLE PRECISION, and are not part of the general parameters or grid parameters indicated in section 5.1). When the parameters are linked to variable arrays, it is possible to define the range of indices that are affected by the SCAN command, e.g., AOMD (13 : 25) means the indices 13 to 25 for the variable linked to the card AOMD. If no index range is given and the variable is an array, the SCAN command applies to the whole range of indices. The parameter is varied between two limits in a certain number of steps. The program

uses one more value than there are steps for each parameter. For example, the program makes four steps between five values.

Key words can be added to affect the way the parameter values are varied:

- REL: The limits indicate a relative value with respect to the nominal value of the parameter.
- DIF: The limits indicate a difference with respect to the nominal value of the parameter.
- BND: When SCAN commands for more than one parameter include the BND key word, these parameters are varied together. Specifically, the same number of steps are taken for these parameter, and a simulation is performed with all parameters at their first value, then another with all parameters at their second value, etc. (Normally, the program varies the parameters one by one trying all combinations of values.)

Example:

```
!
! Scan ozone total column from -50% to +50% of 300 DU
! in 10 steps.
! First set nominal value to 300 DU
O3_N 300
SCAN O3_N 10 -0.5 0.5          REL DIF
!
! Scan aerosols single scattering albedo (range 1:50)
! from 0.8 to 1.0 in 4 steps.
SCAN AOMD(:50) 4 0.80 1.00
```

5.2.1.3 Atmospheric light-absorbing gas cross-section definition

Light absorption by atmospheric gases is simulated in TUV AQM. The wavelength-dependent absorption cross section is read in data files. Some default data files are provided. The command XSEC allows using other files for defining the absorption cross-section for the gases.

- Command key word: XSEC

Command syntax: XSEC File # Subcommand Values

Description:

XSEC is used to define which files contain cross section data for the light-absorbing gas in the atmosphere, and the way to read them. Every XSEC command

refers to a file identified by the file number (second element of the XSEC command line). The command allows defining the name of the file as well as the corresponding absorbing gas. It is assumed that the data are organized in columns with one or two wavelength columns and one or more columns for the corresponding cross sections. It is possible to indicate which columns contain the wavelengths and cross sections. When cross sections are in more than one column, each column is valid for a temperature that is also defined with the XSEC command. More than one file can refer to the same light-absorbing gas. In this case, each file is usually valid for a given wavelength range that is also indicated with XSEC.

Subcommand:

- Subcommand key word: FNAME

Subcommand syntax: XSEC File # FNAME Gas Filename

Description:

XSEC FNAME is used to define the file name and light-absorbing gas corresponding to a given file number. The gas name is a key word that needs to be recognized. The gas name key words are O2, O3, SO2 and NO2.

Example:

```
XSEC 2 FNAME O3 DATAE1/O3/O3.molina.abs
```

Note: The command XSEC File # FNAME can be used without arguments. In this case, what is kept in memory for the given file number is reset, and no file is read. When the user wants to use less files than the default, it is necessary to reset the unused file number that are active by default.

- Subcommand key word: WLLIM

Subcommand syntax: XSEC File # WLLIM Limits Limit type

Description:

When more than one file contains data, it is assumed the files are valid for different wavelength ranges. For example, the cross sections may be measured at different temperature intervals for different wavelength ranges. XSEC WLLIM is used to define what is the wavelength range of validity for a given file. The limits are two wavelengths (nm), and the limit type is a FORTRAN logical expression defining how the limits are used. There are 8 recognized limit types:

- a.lt.wl.and.wl.lt.b
- a.le.wl.and.wl.lt.b
- a.lt.wl.and.wl.le.b
- a.le.wl.and.wl.le.b
- wl.lt.a.or.b.lt.wl
- wl.le.a.or.b.lt.wl
- wl.lt.a.or.b.le.wl
- wl.le.a.or.b.le.wl

The limit type should be strictly identical to one of the recognized types; however, blank characters do not count and can be included anywhere in the limit type.

Example:

```
XSEC 2 WLLIM 240.5 347.0 a .lt. wl .and. wl .lt. b
```

- Subcommand key word: WLCOL

Subcommand syntax: XSEC File # WLCOL Column 1 Column 2

Description:

XSEC WLCOL is used to define what columns in the given file contain the wavelength data. When only one column is indicated, it is assumed that the corresponding cross section is given at that wavelength. When two columns are indicated, they are assumed to be the limits of a bin for which the corresponding cross-section is given.

Example:

```
XSEC 2 WLCOL 2 3
```

- Subcommand key word: XSCOL

Subcommand syntax: XSEC File # XSCOL Col1 Temp1 ...

Description:

XSEC XSCOL is used to define what columns in the given file contain the cross section data. When only one column is indicated, the cross section is assumed not to depend on temperature. When more columns are indicated, they are assumed to be valid at a given temperature each, and every column number should be followed by the corresponding temperature.

Example:

```
XSEC 2 XSCOL 2 226 3 263 4 298
```

5.2.1.4 Extraterrestrial solar flux definition

The intensity of the extraterrestrial solar flux is the primary input in TUVAQM. The extraterrestrial solar flux spectrum is read in data files. Default data files are provided. The command FLUX allows using other files for defining the extraterrestrial solar flux spectrum.

- Command key word: FLUX

Command syntax: FLUX File # Subcommand Values

Description:

FLUX is used to define which file contains the extraterrestrial solar flux spectrum data, and the way to read it. The command allows defining the name of the file and its syntax. It is assumed that the data are organized in columns with one or two columns for wavelength and one or more for the corresponding extraterrestrial solar flux. It is possible to indicate which columns contain the wavelengths and extraterrestrial solar flux. More than one file can be used to define the extraterrestrial solar flux spectrum. In this case, each file is usually valid for a given wavelength range that is also indicated with FLUX.

- Subcommand key word: FNAME

Subcommand syntax: FLUX File # FNAME Filename

Description:

FLUX FNAME is used to define the file name corresponding to a given file number.

Example:

```
FLUX 1 FNAME DATAE1/SUN/susim_hi.flx
```

Note: The command FLUX File # FNAME can be used without arguments.

In this case, what is kept in memory for the given file number is reset, and no file is read. When the user wants to use less files than the default, it is necessary to reset the unused file numbers that are active by default.

- Subcommand key word: WLLIM

Subcommand syntax: FLUX File # WLLIM Limits Limit type

Description:

When more than one file contains data, it is assumed the files are valid for different wavelength ranges. For example, the solar flux measurements can come from different references for different wavelength ranges. FLUX

WLLIM is used to define what is the wavelength range of validity for a given file. The limits are two wavelengths (nm), and the limit type is a FORTRAN logical expression defining how the limits are used. There are 8 recognized limit types:

- a.lt.wl.and.wl.lt.b
- a.le.wl.and.wl.lt.b
- a.lt.wl.and.wl.le.b
- a.le.wl.and.wl.le.b
- wl.lt.a.or.b.lt.wl
- wl.le.a.or.b.lt.wl
- wl.lt.a.or.b.le.wl
- wl.le.a.or.b.le.wl

The limit type should be strictly identical to one of the recognized types; however, blank characters do not count and can be included anywhere in the limit type.

Example:

```
FLUX 1 WLLIM 0 350 a .lt. wl .and. wl .le. b
```

- Subcommand key word: WLCOL

Subcommand syntax: FLUX File # WLCOL Column 1 Column 2

Description:

FLUX WLCOL is used to define what columns in the given file contain the wavelength data. When only one column is indicated, it is assumed that the corresponding solar flux is given at that wavelength. When two columns are indicated, they are assumed to be the limits of a bin for which the corresponding solar flux is given.

Example:

```
FLUX 1 WLCOL 1
```

- Subcommand key word: WLMUL

Subcommand syntax: FLUX File # WLMUL Factor

Description:

FLUX WLMUL defines a wavelength factor for use when the wavelengths are not given in the library routine units (nm). The multiplicative factor is to be applied to all wavelength input from the given file.

Example (units are microns):

```
FLUX 3 WLMUL 1000.0
```

- Subcommand key word: FXCOL

Subcommand syntax: FLUX File # FXCOL Coll Temp1 ...

Description:

FLUX FXCOL is used to define what columns in the given file contain the cross section data. When only one column is indicated, it is assumed that the solar flux is given at the wavelength corresponding to the current line. When more columns are indicated, it is assumed that each column gives flux values at a wavelength with a given offset from the base wavelength given for each line (a different offset for each column allows reducing the number of lines to be read for high resolution files). Every column number should be followed by the corresponding offset.

Example:

```
FLUX 3 FXCOL 2 .00 3 .05 4 .10 5 .15 6 .20 7 .25
```

- Subcommand key word: FXMUL

Subcommand syntax: FLUX File # FXMUL Factor Flag

Description:

FLUX FXMUL defines a solar flux factor for use when the file solar flux is not given in the library routine units ($\text{watts m}^{-2} \text{nm}^{-1}$). The multiplicative factor is to be applied to all solar flux inputs from the given file. A logical flag can be given to indicate when the solar flux is given as energy quanta. In this case, to obtain the solar flux in the working units, TUVAQM divides the flux by the wavelength.

Example (solar flux given as light quanta):

```
FLUX 2 FXMUL 1.985E-12 .TRUE.
```

- Subcommand key word: INTSC

Subcommand syntax: FLUX File # INTSC Interp. scheme

Description:

FLUX INTSC allows choosing the scheme to be used to interpolate the solar flux data from the wavelength grid indicated in the file to the general wavelength grid. Three interpolation schemes are possible:

- 1) The original input data are given on single, discrete points of an arbitrary grid and are linearly interpolated onto the specified discrete target grid. A typical example would be the re-gridding of a given data set for the vertical temperature profile to match the specified altitude grid.
- 2) The original input data are given on single, discrete points of an arbitrary grid and are linearly interpolated onto a specified set of target bins. In general, this is the case for most of the weighting functions (action spectra, molecular cross section, and quantum yield data) which have to be matched onto the specified wavelength intervals. The average value in each target bin is found by averaging the trapezoidal area underneath the input data curve (constructed by linearly connecting the discrete input values).
- 3) The input data are given on a set of bins representing the input quantity integrated over the range of each bin (the area of each bin) and are matched onto another set of bins (target grid). The resulting area in a given bin of the target grid is calculated by simply adding all fractional areas of the input data that cover that particular target bin.

Example (solar flux given as light quanta):

FLUX 1 INTSC 2

5.2.1.5 Photolysis reaction cross section and quantum yield definition

TUVAQM computes the solar irradiance in the atmosphere. It can be used to compute the photolysis reaction rate coefficient (in sec^{-1}) for given reactions, providing the corresponding cross-sections and quantum yields are known. The cross sections and quantum yields are read in data files. Currently, TUVAQM reads cross-sections and quantum yields for 20 photolysis reactions defined in SAPRC97 (<http://cert.ucr.edu/~carter/saprc97.htm>). The SAPRC97 reactions are:

1	1	NO ₂	NO ₂ + hv \Rightarrow NO + O
2	12A	NO ₃	NO ₃ + hv \Rightarrow NO + O ₂
3	12B	NO ₃	NO ₃ + hv \Rightarrow NO ₂ + O
4	13A	Ozone	O ₃ + hv \Rightarrow O + O ₂
5	13B	Ozone	O ₃ + hv \Rightarrow O*1D2 + O ₂

6	17	HONO	$\text{HONO} + h\nu \Rightarrow \text{HO}_2 + \text{NO}$
7	31	H_2O_2	$\text{HO}_2\text{H} + h\nu \Rightarrow 2 \text{HO}_2$
8	B7	CO_2H	$-\text{OOH} + h\nu \Rightarrow \text{HO}_2 + \text{HO}_2$
9	C1	HCHO	$\text{HCHO} + h\nu \Rightarrow 2 \text{HO}_2 + \text{CO}$
10	C2	HCHO	$\text{HCHO} + h\nu \Rightarrow \text{H}_2 + \text{CO}$
11	C11A	CCHO	$\text{CCHO} + h\nu \Rightarrow \text{CO} + \text{HO}_2 + \text{HCHO} + \text{RO}_2\text{-R} + \text{RO}_2$
12	C26	RCHO	$\text{RCHO} + h\nu \Rightarrow \text{CCHO} + \text{RO}_2\text{-R} + \text{RO}_2 + \text{CO} + \text{HO}_2$
13	C39	Acetone	$\text{ACET} + h\nu \Rightarrow \text{CCO-O}_2 + \text{HCHO} + \text{RO}_2\text{-R} + \text{RCO}_3 + \text{RO}_2$
14	C57	MEK	$\text{MEK} + h\nu + 0.1 \Rightarrow \text{CCO-O}_2 + \text{CCHO} + \text{RO}_2\text{-R} + \text{RCO}_3 + \text{RO}_2$
15	C58A	Glyoxal	$\text{GLY} + h\nu \Rightarrow 0.8 \text{HO}_2 + 0.45 \text{HCHO} + 1.55 \text{CO}$
16	C58B	Glyoxal	$\text{GLY} + h\nu + 0.029 \Rightarrow 0.13 \text{HCHO} + 1.87 \text{CO}$
17	C68A	Methyl-Glyoxal	$\text{MGLY} + h\nu \Rightarrow \text{HO}_2 + \text{CO} + \text{CCO-O}_2 + \text{RCO}_3$
18	C68B	Methyl-Glyoxal	$\text{MGLY} + h\nu + 0.107 \Rightarrow \text{HO}_2 + \text{CO} + \text{CCO-O}_2 + \text{RCO}_3$
19	G31	Benzaldehyde	$\text{BALD} + h\nu + 0.05 \Rightarrow 7 \text{-C}$
20	G8	Acrolein	$\text{AFG1} + h\nu + 0.077 \Rightarrow \text{HO}_2 + \text{HCOCO-O}_2 + \text{RCO}_3$
21	U2HV	Acrolein	$\text{AFG2} + h\nu \Rightarrow \text{HO}_2 + \text{CO} + \text{CCO-O}_2 + \text{RCO}_3$

Note: reaction 20 (G8) and 21 (U2HV) use the same cross section and quantum yield definition and only the rate coefficient for reaction 20 is computed.

No command is installed yet to allow choosing the reactions. Code changes are needed to implement a different set of reactions (see section 8).

6 Region and time-dependent card description

The region and time-dependent card input file indicates the value of the parameters assumed to vary with time and space (see section 3). These parameters correspond to parameters defined with cards in section 5 (latter referred to as general cards). Within an AQM, the library routines use the values read in the region and time-dependent card input files to substitute for the default values (or the values set with general cards) with the appropriate values for the current region and time interval. A list of the parameters that are modified and the corresponding general cards is given below:

zenith angle	LTIM, NSTO, SPNT	LTIM is set to <code>.FALSE.</code> , NSTO is set to the number of zenith angles requested for the region and time interval, and SPNT is set to the zenith angle values.
elevation grid	NBZG, ZGRD	NBZG is set to the number of elevation levels requested for the region and time interval, and ZGRD is set to the elevation level values.
ground albedo	ALNW, ALWG, ALBD	ALNW is set to 1, ALWG is set to one wavelength bin covering the whole wavelength range, and ALBD is set to the ground albedo value requested for the region.
total ozone column	O3_N	O3_N is set to the total ozone column requested for the region and time interval.
total aerosol optical depth	AERF, AODN	AERF is set to <code>.TRUE.</code> , and AODN is set to the total aerosol optical depth requested for the region and time interval.
aerosol single scattering albedo	AOMD	AOMD is set to the single scattering albedo requested for the region and time interval.
aerosol asymmetry factor	AGDE	AGDE is set to the asymmetry factor requested for the region and time interval.

The syntax of the region and time-dependent card input file is similar to the syntax of general card and command input files. However, there are more restrictions: no elements of the file can be skipped, and the elements should appear in a definite order. Because of these differences, to avoid confusion, the key words in the region and time-dependent card input file are different from

the corresponding key words of the general card and command input file. All inputs in the file take the form of one key word followed by the corresponding values, possibly on several lines, until the next key word. Values are separated by one or more blank characters or tabulation characters. In order to increase the readability of the input file, comment lines starting with an exclamation mark can be included at any time. The sequence of information in the region and time-dependent card input file is the following:

1. Number of regions and time interval limits

When using TUVAQM within an AQM, the user must divide the modeling domain in regions and the modeling episode in time intervals such that the atmospheric properties are relatively constant in a given region and time interval. The number of regions and time interval limits is given here. Note: since the time interval *limits* are given here, there should be one more limit than there are time intervals.

Key word: NBRT

Syntax: NBRT Number of regions Number of time limits

Example: NBRT 2 4

2. Time interval limits

The time interval limits are given in the AQM working time units (usually in minutes). The limits measure the simulated time elapsed since the beginning of the simulation. They should be in a strictly ascending order. There should be as many limits as declared with NBRT.

Key word: TINT

Syntax: TINT Limit 1 Limit 2 Limit 3...

Example: TINT 0 240 480 720

3. Number of ground elevations per region

In each region, the ground elevation may vary substantially. When used within an AQM, TUVAQM computes simulations for a certain number of ground elevations that are representative for the region. The results for a given AQM cell with a given ground elevation are interpolated from the results of the simulations with the representative ground elevations. The number of representative ground elevations for each region is set with NGEL. There should be as many numbers as there are regions (defined with NBRT). The interpolation is done with a 3-points 2nd-order polynomial algorithm; thus, there should be at least 3 representative ground elevations per region.

Key word: NGEL

Syntax: NGEL # of elevation 1 # of elevation 2
of elevation 3...

Example: NGEL 4 3

4. Ground elevations in each region

The representative ground elevations in each region are given in the units of the general elevation grid, that is kilometers above sea level (*not meters above sea level*). GREL is the key word indicating the ground elevation input. It should be repeated as many time as there are regions, and for each region there should be as many inputs as declared with NGEL. Each series of ground elevations should be in a strictly ascending order.

Key word: GREL

Syntax: GREL Elevation 1 Elevation 2 Elevation 3...

Example: ! Region 1

GREL 0.0 0.5 1.0 1.5

! Region 2

GREL 0.2 0.6 1.0

5. Number of zenith angle steps per region and time interval

The solar zenith angle depends on the location, date and time. Since time intervals can be defined as lasting several hours, the solar zenith angle may change significantly within a time interval. In case the modeling domain is very large, the zenith angle range for a given time interval may also change from one region to the other. Simulations are computed for zenith angles representative for each region and time interval. The results at a given time for a given AQM cell resulting in a given zenith angle are interpolated from the results of the simulations with the representative zenith angles. The number of representative zenith angles for each region and time interval is set with NBZN. It should be repeated as many times as there are regions, and for each region there should be as many inputs as there are time intervals. The interpolation is done with a 3-points 2nd-order polynomial algorithm; thus, there should be at least 3 representative zenith angles per region and time interval.

Key word: NBZN

Syntax: NBZN # of zenith angles 1 # of zenith angles 2
of zenith angles 3...

Example: ! Region 1 (3 time intervals)

NBZN 8 5 8

! Region 2 (3 time intervals)

NBZN 8 4 8

6. Zenith angle steps in each region and time interval

The representative solar zenith angle steps in each region and time interval are given in degrees. ZNST is the key word indicating the zenith angle input. It should be repeated as many times as there are regions multiplied by time intervals, and for each region and time interval there should be as many inputs as declared with NBZN. Each series of zenith angles should be in a strictly ascending order *even though the solar zenith angle decreases during the afternoon*.

Key word: ZNST

Syntax: ZNST Zenith angle 1 Zenith angle 2 Zenith angle 3...

Example: !

```
!      Region 1 (3 time intervals with 8, 5 and 8 steps)
ZNST 40 50 60 70 75 80 85 90
ZNST 0 10 20 30 40
ZNST 40 50 60 70 75 80 85 90
!
!      Region 2 (3 time intervals with 8, 4 and 8 steps)
ZNST 40 50 60 70 75 80 85 90
ZNST 10 20 30 40
ZNST 40 50 60 70 75 80 85 90
```

7. Number of levels in elevation grid per region and time interval

TUVAQM uses one general elevation grid for performing the radiation transfer calculations. This grid is user-defined. All quantities that depend on elevation are given a fixed value in each cell of the general elevation grid. The choice of the elevation grid should depend on the altitude resolution of the input data (air pressure, aerosol and absorbing gas density, etc.) and the expected resolution of the output. The different inputs are all given on their own elevation grid, and library routines map them on the general grid. Thus, having a grid with smaller cells than the cells of the finest input grid does not improve the precision of the calculation. Similarly, the AQM callable routine of TUVAQM maps the results computed on the general grid to the desired output grid. Thus, a general grid with cells larger than the output grid will lead to a loss of resolution. For each region and time interval a specific elevation grid is defined. The number of levels in the elevation grid for each region and time interval is set with NBHL. It should be repeated as many time as there are regions, and for each region there should be as many inputs as there are time intervals.

Key word: NBHL

Syntax: NBHL # of altitude levels 1 # of altitude levels 2
of altitude levels 3...

Example: ! Region 1 (3 time intervals)

NBHL 34 32 30

! Region 2 (3 time intervals)

NBHL 32 32 31

8. Elevation grid levels in each region and time interval

The levels of the general elevation grid are given with the key word HLEV. Since different ground elevations can be defined for the same region, the elevation grid is defined relative to the ground elevation level, and not from the sea level. The levels are given *in kilometers above ground level*. The bottom of the lowest cell is always assumed to be the ground level. Thus the first elevation level is the top of the first cell. Consequently, the number of elevation levels (see NBHL) is equal to the number of cells in the elevation grid. The HLEV key word should be repeated as many times as there are regions multiplied by time intervals, and for each region and time interval there should be as many inputs as declared with NBHL. Each series of elevations should be in a strictly ascending order.

Key word: HLEV

Syntax: HLEV Elevation 1 Elevation 2 Elevation 3...

Example: !

! Defines elevation levels in each region and

! time interval

! Region 1 (3 time intervals with 34, 32 & 30 levels)

HLEV 0.1 0.2 0.3 0.4 0.5 1.0 2.0 3.0 4.0 5.0 8.0 12.0
13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24.
25. 26. 27. 28. 29. 30. 35. 40. 45. 50.

HLEV 0.1 0.3 0.5 1.0 2.0 3.0 4.0 5.0 8.0 12.0
13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24.
25. 26. 27. 28. 29. 30. 35. 40. 45. 50.

HLEV 0.1 0.3 0.5 1.0 2.0 3.0 5.0 12.0
13. 14. 15. 16. 17. 18. 19. 20. 21. 22. 23. 24.
25. 26. 27. 28. 29. 30. 35. 40. 45. 50.

```

!
! Region 2 (3 time intervals with 32, 32 & 31 levels)
HLEV  0.1 0.25 0.5 1.0 2.0 3.0 4.0 5.0 8.0 12.0
      13. 14. 15. 16. 17. 18. 19. 20.
      21. 22. 23. 24. 25. 26. 27. 28. 29. 30.
      35. 40. 45. 50.
HLEV  0.1 0.25 0.5 1.0 2.0 3.0 4.0 5.0 8.0 12.0
      13. 14. 15. 16. 17. 18. 19. 20.
      21. 22. 23. 24. 25. 26. 27. 28. 29. 30.
      35. 40. 45. 50.
HLEV  0.1      0.5 1.0 2.0 3.0 4.0 5.0 8.0 12.0
      13. 14. 15. 16. 17. 18. 19. 20.
      21. 22. 23. 24. 25. 26. 27. 28. 29. 30.
      35. 40. 45. 50.

```

9. Ground albedo in each region

An average ground albedo (a single value valid at all wavelengths) can be defined for each region. The GALB key word should be given with as many inputs as there are regions.

Key word: GALB

Syntax: GALB Ground albedo 1 Ground albedo 2 Ground albedo 3...

Example: !

```

! Average ground albedo in each region
GALB  0.08 0.20

```

10. Total ozone column in each region and time interval

The total ozone column is one of the important atmospheric properties that should be defined separately for each region and time interval. The total ozone column is given in Dobson units with the O3TC key word. It should be repeated as many time as there are regions, and for each region there should be as many inputs as there are time intervals.

Key word: O3TC

Syntax: O3TC O₃ column 1 O₃ column 2 O₃ column 3...

Example: !

```

! Gives O3 total ozone column in each region and
! time interval
!
! Region 1 (3 time intervals)
O3TC  305.0 300.3 302.5

```

```

!
! Region 2 (3 time intervals)
O3TC  298.6 300.3 300.2

```

11. Aerosol properties in each region and time interval

Average atmospheric aerosol properties that should be defined separately for each region and time interval are the aerosol total optical depth, the aerosol single scattering albedo and the aerosol asymmetry factor. The aerosol total optical depth is given in form of attenuation factor per kilometer of atmosphere. It is used to scale the atmospheric aerosol optical depth profile (either the default one or the one defined as discussed in section 5). The single scattering albedo and asymmetry factor are average quantities that apply to all altitude cells. (It was assumed that data on their elevation profile were too scarce to warrant a more precise definition). The key word for total optical depth is ATOD, AOME for the single scattering albedo, and AGDE for the asymmetry factor. These key words should be given one after the other as many times as there are regions, and should each have as many inputs as there are time intervals.

Key word: ATOD, AOME, AGDE

Syntax: ATOD Optical depth 1 Optical depth 2 Optical depth 3...
AOME S.s. albedo 1 S.s. albedo 2 S.s. albedo 3...
AGDE Asym. fact. 1 Asym. fact. 2 Asym. fact. 3...

Example: !
! Aerosol properties in each region and time interval
!
! Region 1 (3 properties for 3 time intervals)
ATOD 0.5 1.0 0.7
AOME 0.90 0.80 0.85
AGDE 0.61 0.66 0.61
! Region 2 (3 properties for 3 time intervals)
ATOD 0.1 0.3 0.3
AOME 0.90 0.90 0.90
AGDE 0.61 0.61 0.61

7 Installing TUV AQM

The library routines are written in FORTRAN 77. The library routine package is distributed as an archive file created with the UNIX tar utility and compressed with UNIX gzip. On most UNIX system, the archived compressed file can be uncompressed with the command

gunzip tuvaqm.tar.zip, and de-archived with the command `tar -xf tuvaqm.tar`. At the upper level, the archive file contains two UNIX directories and a Readme file describing the directories. The first directory called Dcode contains the FORTRAN code for the library routines. The second directory called Drun contains supporting files needed for most radiation transfer simulations. When the code is compiled and an executable created, it should be run within Drun, because supporting file names are given as relative paths and not absolute paths. It is also possible to create an object library containing the main AQM-callable routine (subroutine tuvaqm) and the other library routines. Any executable calling tuvaqm will need the supporting data within Drun.

With the code is included a makefile for the UNIX make utility. The makefile includes several targets (entry points). The main target (tuvlib.a) is used for creating the object library containing the main AQM-callable routine and the library routines. Hence the command `make` or `make tuvlib.a` issued within the directory Dcode will create the object library `tuvlib.a` that can be linked with an AQM program calling tuvaqm. The other targets are used to create standalone executables using the library routines. The name of the executable created is identical to the target. For example, the command `make t_taqm` will create the executable `t_taqm`. These executables differ in the main program used, and the output package used. `t_taqm` and `t_taqmh` use a main program that tests the library routines with a calling sequence similar to what an AQM would use. `t_tuvn`, `t_tuvh` and `t_tuvw` use a main program that only performs one radiation transfer simulation. `s_tuvn`, `s_tuvh` and `s_tuvw` use a main program that allows rerunning the radiation transfer model while varying desired input parameters. `t_tuvn` and `s_tuvn` do not save results, whereas `t_tuvh` and `s_tuvh` save photolysis reaction rate coefficient results in a format described as CERN RZ libraries (<http://wwwinfo.cern.ch/asdoc/>, the CERN libraries are needed only for these two executables). `t_tuvw` and `s_tuvw` save the results with simple FORTRAN write statements.

The makefile uses the standard FORTRAN compiler (variable FC). On most UNIX operating systems this is defined as `f77`. However, it may not be available on some system, and FC may not be defined appropriately. Such a problem can occur on LINUX systems where one can try to define `FC = g77`, or on systems featuring only the newer `f90` where defining `FC = f90` should solve the problem.

Use of TUVAQM can be computationally intensive, especially when it is called repeatedly. To lower the computational burden, it is a good idea to use the code optimization utility available with most compilers. The original version of the makefile uses compilation flags (variable FFLAGS) that produce aggressive optimization on a SUN Sparc station without use of

multiprocessing. These flags usually depend on the compiler and the operating system, and it is up to the user to find the appropriate flags.

In the directory `Drun`, some input and output files are provided so that the user can check that the desired executables are correctly installed. A `Readme` file in the directory describes its content.

8 Code description

SUBROUTINE `TUVAQM` (in file `tuvaqm.f`) is the only routine that should be called from an Air Quality Model. It uses seven generic routines that perform a group of related tasks. The seven generic routines call numerous other routines that perform a single task each. While the seven generic routines are each contained in separate files, the other supporting routines are grouped into files according to their purpose. In addition there are four test main programs.

Beside `TUVAQM`, the seven generic routines are `DEP_RD`, `GETPAR`, `GTPLOC`, `MODPAR`, `TUV_RD`, `TUV_RN` and `ZG_MOD` (files `dep_rd.f`, `getpar.f`, `gtploc.f`, `modpar.f`, `tuv_rd.f`, `tuv_rn.f` and `zg_mod.f`, respectively). All these routines are thoroughly documented.

8.1.1 Generic routines

8.1.1.1 `tuvaqm.f`

`TUVAQM` is a general main routine for using TUV within an AQM program. `TUVAQM` should be called once at initialization time, and then it should be called every time J values are needed for the photolysis reactions. `TUVAQM` provides the J-values for all reactions defined at the initialization step, for all cells in a column defined in the calling sequence.

Content:

SUBROUTINE `TUVAQM`: Radiative transfer initialization or computation.

8.1.1.2 `dep_rd.f`

`DEP_RD` is a routine that reads the user's defined radiative transfer atmospheric properties for each AQM time interval and region.

Content:

SUBROUTINE `DEP_RD`: Reads time interval and region definition.

8.1.1.3 getpar.f

GETPAR is a routine that gets the value of a parameter (e.g. total ozone column) or an array of parameters whose position in the general parameter array has previously been identified by subroutine GTPLOC.

Content:

SUBROUTINE GETPAR: Retrieves the value of parameters identified by gtploc.

8.1.1.4 gtploc.f

GTPLOC is a routine that returns the location of a given parameter (e.g. total ozone column) in the parameter array based on the datacard name linked to the parameter (in the case of total ozone column, the datacard name is O3_N). GTPLOC should be called at the beginning of the program once for each parameter that will need to be updated during execution.

Content:

SUBROUTINE GTPLOC: Finds the variable pertaining to a given input parameter.

8.1.1.5 modpar.f

MODPAR is a routine that modifies the value of a parameter (or a parameter array). The parameter is identified by the location returned from GTPLOC. MODPAR should be called before the routine computing the J-values (TUV_RN), once for each parameter modified since the last execution of TUV_RN.

Content:

SUBROUTINE MODPAR: Modify an input parameter or an array of input parameters.

8.1.1.6 tuv_rd.f

TUV_RD is an initialization routine that reads user's directives and various data files. It should be called once at the beginning of the program.

Content:

SUBROUTINE TUV_RD: Performs general initialization and reads data file.

8.1.1.7 tuv_rn.f

TUV_RN is the routine simulating the radiation transfer, and computing the J-values.

Content:

SUBROUTINE TUV_RN: Sets up model atmosphere and calls the radiation transfer routine.

8.1.1.8 zg_mod.f

ZG_MOD is a routine that modifies the bottom part of the altitude grid, so that the lower part of the TUVAQM general z-grid corresponds to the AQM z-grid. ZG_MOD should be called before the routine computing the J-values (TUV_RN), if the AQM z-grid was modified since the last execution of TUV_RN.

Content:

SUBROUTINE ZG_MOD: Modifies the altitude grid to incorporate new layers.

8.1.2 Test programs

8.1.2.1 mn_try.f

File mn_try.f contains a test program using the routines described above.

Content:

MAIN MN_TUV: Main program to test the subroutines described above.

8.1.2.2 mn_sca.f

File mn_sca.f contains a program that allows rerunning a radiation transfer simulation while changing the value of desired input parameters step by step.

Content:

MAIN MN_TUV: Main program used for TUVAQM with input parameter value scan.

SUBROUTINE SCAVAL: Runs TUV_RN repeatedly while changing input parameter values.

8.1.2.3 tstaqm.f

File tstaqm.f contains a test program that uses TUVAQM in a calling sequence that emulates the one that could be found in an AQM.

Content:

MAIN TSTAQM: Main program used for testing TUVAQM in AQM calling sequence.

8.1.2.4 tstaqmh.f

File tstaqmh.f is identical to tstaqm.f except that CERN libraries are used for saving the program outputs.

Content:

MAIN TSTAQM: Main program used for testing TUVAQM in AQM calling sequence.

8.1.3 Other routines

8.1.3.1 setsca.f

When the program in mn_sca.f is chosen, setsca is used to choose what parameters are varied, and what are the values at each step.

Content:

SUBROUTINE SETSCA: Set initial values for a scan of possible parameter values.
BLOCK DATA BDSCAN: Initializes default data for parameter value scanning.

8.1.3.2 caread.f

File caread.f contains routines used to set and show values for parameters describing how the radiative transfer simulation should proceed.

Content:

SUBROUTINE CARINI: Initializes the parameter value input package.
SUBROUTINE CAREAD: Reads and interprets the lines of the parameter value file.
SUBROUTINE CARINP: Inputs one line of the parameter value file.
SUBROUTINE CAINCA: Interprets values for simple parameter definitions.
SUBROUTINE CAINCO: Interprets command lines.
FUNCTION LENOCC: Finds the last non-blank character of a string.
FUNCTION LVCATS: Finds a character string in a character string array.
SUBROUTINE LVUPCA: Changes the case of a character string to uppercase.
SUBROUTINE CARSHS: Shows current status of user's input cards
SUBROUTINE CARSH1: Shows current status of one of the user's input cards
SUBROUTINE CARSHL: Writes a string of logical data
SUBROUTINE CARSHI: Writes a string of integer data
SUBROUTINE CARSHR: Writes a string of real data
SUBROUTINE CARSHD: Writes a string of double precision data
SUBROUTINE CARSHC: Writes character strings data

8.1.3.3 inidef.f

File inidef.f contains a group of BLOCK DATA that gives default values to the parameters set by the code in caread.f

Content:

BLOCK DATA CARDEF: Defines keywords used for initializing parameters.
BLOCK DATA CARVAL: Gives default values for user-defined parameters.
BLOCK DATA CMDDEF: Defines keywords for initialization commands.
BLOCK DATA BDFXRD: Defines subcommands for reading solar flux data files.
BLOCK DATA BDXSRD: Defines subcommands for reading cross-section data files.

8.1.3.4 setcnd.f

File setcnd.f contains routines that set-up the environment conditions for simulating the radiative transfer once the parameters describing the environment conditions have been read.

Content:

SUBROUTINE SETAER: Sets up an altitude profile for aerosol characteristics.
SUBROUTINE SETAIR: Sets up an altitude profile for air density.
SUBROUTINE SETALB: Sets up a wavelength profile for ground albedo.
SUBROUTINE SETCLD: Sets up an altitude profile for cloud characteristics.
SUBROUTINE SETNO2: Sets up an altitude profile for NO₂ absorption optical depth.
SUBROUTINE SETO2: Sets up an altitude profile for O₂ absorption optical depth.
FUNCTION FCHAP: Computes the Chapman function (O₂ absorption optical depth).
SUBROUTINE SCHU: Computes equivalent O₂ absorption x-section in SR bands.
SUBROUTINE SETOZO: Sets up an altitude profile for O₃ absorption optical depth.
SUBROUTINE SETSO2: Sets up an altitude profile for SO₂ absorption optical depth.
SUBROUTINE SETTMP: Sets up an altitude profile for temperature.

8.1.3.5 setphr.f

File setphr.f contains code to define weighting functions for the photolysis reactions of interest. The radiative transfer simulation computes the wavelength-dependent irradiance at a given time and location. To compute photolysis reaction rate coefficients, wavelength-dependent cross sections and quantum yields need to be known. The weighting functions are defined as the product of the cross section times the quantum yield.

Content:

SUBROUTINE RDPHOD: Reads the weighting functions information.
FUNCTION NBARG: Returns the number of arguments in a character string.
SUBROUTINE SETPHO: Computes the weighting functions for photolysis reactions.

8.1.3.6 setflx.f

File setflx.f contains code for inputting the extraterrestrial (solar) flux. The extraterrestrial flux (mainly from solar radiation) is the source of all the primary radiation. It is a wavelength-dependent quantity read in one or more data files.

Content:

```
SUBROUTINE RDXFXFI: Reads extraterrestrial (solar) flux data files.
SUBROUTINE SETFXR: Sets characteristics for reading solar flux data files.
SUBROUTINE SFXFXC: Gets solar flux data file format for solar flux definition.
SUBROUTINE SFXFXM: Gets a multiplicative factor for solar flux definition.
SUBROUTINE SFXINS: Gets an interpolation scheme number for wavelengths.
SUBROUTINE SFXLIM: Gets wavelength validity domain for solar flux data files.
SUBROUTINE SFXNAM: Gets extraterrestrial (solar) flux file names.
SUBROUTINE SFXWLC: Gets solar flux data file format for wavelength definition.
SUBROUTINE SFXWLM: Gets a multiplicative factor for wavelength definition.
```

8.1.3.7 setxsn.f

File setxsn.f contains the code to define the absorption cross section (x-section) for different gases. Gases in the atmosphere absorb radiation. The absorption cross sections for the main absorbing gases in the atmosphere are read in data files.

Content:

```
SUBROUTINE RDXSFI: Reads gas absorption x-section files.
SUBROUTINE SETXSR: Sets characteristics for reading gas absorption x-sections.
SUBROUTINE SXSLIM: Gets wavelength validity domain for x-section data files.
SUBROUTINE SXSNAM: Gets gas absorption x-section file names.
SUBROUTINE SXSWLC: Gets x-section data file format for wavelength definition.
SUBROUTINE SXSXSC: Gets x-section data file format for x-section definition.
```

8.1.3.8 tuvgrd.f

File tuvgrd.f contains the code to define the altitude and wavelength general grid. All quantities that depend on the altitude or the wavelength are defined on grids. The user can define the grids. Most radiation quantities are wavelength dependent. Quantities that depend on temperature or pressure are altitude (elevation) dependent.

Content:

SUBROUTINE GRIDCK: Checks grid for correct structure.
SUBROUTINE GRIDW: Sets wavelength general grid.
SUBROUTINE GRIDZ: Sets altitude (elevation) general grid.

8.1.3.9 rad_tr.f

File rad_tr.f contains the code that performs the radiation transfer simulation once the environment conditions are set.

Content:

SUBROUTINE PS2STR: Computes 2 stream radiative transfer approximation.
SUBROUTINE TRIDAG: Solves tridiagonal matrix system.
SUBROUTINE RTLINK: Transforms data to the desired format, then call ps2str.

8.1.3.10 tuvutl.f

File tuvutl.f contains utility routines that compute some general quantity or perform some general manipulation on data.

Content:

SUBROUTINE ADDPNT: Adds a point in a pair of related ordered grids.
SUBROUTINE ADMPNT: Adds multiple points in a pair of related ordered grids.
FUNCTION FSUM: Sums values in an array.
SUBROUTINE INTER1: Interpolates data given on one grid on another grid.
SUBROUTINE INTER2: Idem
SUBROUTINE INTER3: Idem
SUBROUTINE SPHERS: Computes slant path over vertical depth in spherical geom.
SUBROUTINE SUNDIS: Computes Earth-Sun distance variation for a given date.
SUBROUTINE ZENITH: Computes solar zenith and azimuth for a given date/place.
SUBROUTINE ZERO1: Initializes a 1-dim array with zeros.
SUBROUTINE ZERO2: Initializes a 2-dim array with zeros.
FUNCTION LOCREA: Locates where a real values stands in an ordered list.
SUBROUTINE JINTER: Computes J-value by interpolation from previously computed values
SUBROUTINE INTPOL: Performs a 2nd-order polynomial 3-points interpolation.
SUBROUTINE GTNGRP: Reads a group of lines giving all values for a given a variable.
SUBROUTINE GTNLIN: Reads a group of values on a line.
SUBROUTINE SPLLIN: Splits a line in elements.

8.1.3.11 outpaw.f

File outpaw.f contains code to save results in a database format defined by the CERN (European Organization for Particle Physics) computer libraries. The format is the RZ HBOOK n-tuple format. (See <http://wwwinfo.cern.ch/asdoc/>).

Content:

SUBROUTINE FORPAW: Saves results on an HBOOK-type database (CERN libraries).

SUBROUTINE TRADAT: Aggregates all results in a single COMMON for HBOOK.

8.1.3.12 tuvold.f

File tuvold.f contains code that defines photolysis reaction weighting functions in the original TUV code by Sasha Madronich. It is not used in this version.

Literature cited

- Baldasano J. M., Delgado R. and Calbo J., 1998. Applying receptor models to analyze urban/suburban VOCs air quality in Martorell (Spain). *Environ. Sci. Technol.* 32, 405-412.
- Bergin M. S., Russell A. G. and Milford J. B., 1998. Effects of chemical mechanism uncertainties on the reactivity quantification of volatile organic compounds using a three-dimensional air quality model. *Environ. Sci. Technol.* 32, 694-703.
- Bigelow D. S. and Slusser J. R., 2000. Establishing the stability of multi-filter UV rotating shadowband radiometers. *J. Geophys. Res.* 105, 4833-4840.
- Bigelow, D. S., Slusser J. R., Beaubien A. F. and Gibson J. H., 1998. The USDA Ultraviolet Radiation Monitoring Program. *Bull. Amer. Meteorol. Soc.* 79, 601-615.
- Blindauer C., Rozanov V. and Burrows J. P., 1996. Actinic flux and photolysis frequency comparison computations using the model PHOTOGT. *J. Atmos. Chem.* 24, 1-21.
- Carter W. P. L. Updated SAPRC-97 Mechanism. Electronic source at <ftp://cert.ucr.edu/pub/carter/mech/saprc97/>, 1997.
- Chandrasekhar, S. Radiative transfer. Dover, New York, 1960 (2nd ed.) 393pp.
- Coakley J. A. Jr. and Chýlek P., 1975. The two-stream approximation in radiative transfer: Including the angle of the incident radiation. *J. Atmos. Sci.* 32, 409-418.
- Demerjian K.L., Schere K.L. and Peterson J.T., 1980. Theoretical estimates of actinic (spherically integrated) flux and photolytic rate constants of atmospheric species in the lower troposphere. In *Advances in Environmental Science and Technology*, 10, 369-441.
- Dickerson R. R., Kondragunta S., Stenchikov G., Civerto K. L., Doddridge B. G. and Holben B. N., 1997. The impact of aerosols on solar ultraviolet radiation and photochemical smog. *Science* 278, 827-830.
- Elterman L. UV, Visible and IR Attenuation for Altitude to 50 km. Report AFCRL-68-0153 ERP 285, Air Force Cambridge Research Laboratories, Bedford, MA, 1968.
- Everitt B. S. and Dunn G. *Applied Multivariable Data Analysis*. Oxford University Press, New York, NY, 1992.
- Falls A. H., McRae G. J. and Seinfeld J. H., 1979. Sensitivity and uncertainty of reaction mechanisms for photochemical air pollution. *Int. J. Chem. Kinet.* 11, 1137-1162.

- Finlayson-Pitts B. J. and Pitts J. N. Jr. Atmospheric Chemistry: Fundamentals and Experimental Techniques. Wiley-Interscience, New York, NY, 1986.
- Gao D., Stockwell W. R. and Milford J. B., 1995. First-order sensitivity and uncertainty analysis for a regional-scale gas-phase chemical mechanism. *J. Geophys. Res.* 100, 23153-23166.
- Gao D., Stockwell W. R. and Milford J. B., 1996. Global uncertainty analysis of a regional-scale gas-phase chemical mechanism. *J. Geophys. Res.* 101, 9107-9119.
- Gery M. W., Whitten G. Z., Killus J. P. and Dodge M. C., 1992. A Photochemical Kinetics Mechanism for Urban and Regional Scale Computer Modeling. *J. Geophys. Res.* 94, 12,925–12,956.
- Harley R. A., Russell A. G., McRae G. J., Cass G. R. and Seinfeld J. H., 1993. Photochemical modeling of the Southern California Air Quality Study. *Environ. Sci. Technol.*, 27, 378-388.
- Harrison L. and Michalsky J., 1994. Objective algorithms for the retrieval of optical depths from ground-based measurements. *Appl. Opt.* 33, 5126-5132.
- Henry R. C. and Hidy G. M., 1979. Multivariate analysis of particulate sulfate and other air quality variables by principal components — Part I. Annual data from Los Angeles and New York. *Atmos. Environ.* 13, 1581-1596.
- Henry R. C. and Hidy G. M., 1982. Multivariate analysis of particulate sulfate and other air quality variables by principal components — Part II. Salt Lake City, Utah and St. Louis, Missouri. *Atmos. Environ.* 16, 929-943.
- Jolliffe I. T., 1972. Discarding variables in a principal component analysis 1: Artificial data. *Applied Statistics* 21 160-173.
- Joseph J. H., Wiscombe W. J. and Weinman J. A., 1976. The delta-Eddington approximation for radiative transfer. *J. Atmos. Sci.* 33, 2452-2459.
- Larson, S., Cass G., Hussey, K., and Luce F., 1984. Visibility model verification by image processing techniques. Final Report to State of California Air Resources Board under Agreement A2-077-32, Sacramento, CA.
- Lean, J. L., Rottman G. J., Kyle H. L., Woods T. N., Hickey J. R., and Puga L. C., 1997. Detection and parameterization of variations in solar middle and near-ultraviolet radiation (200-400 nm). *J. Geophys. Res.* 102, 29,939-29,956.
- Lenoble J. (ed.) Radiative Transfer in Scattering and Absorbing Atmospheres: Standard Computational Procedures. A. Deepak Publishing, Hampton, VA, 1985. 300 pp.

- Liou K.-N., 1973. A numerical experiment on Chandrasekhar's discrete-ordinate method for radiative transfer: Applications to cloudy and hazy atmospheres. *J. Atmos. Sci.* 30, 1303-1326.
- Lurmann F. W., Carter W. P. L. and Coyner L. A. A Surrogate Species Chemical Reaction Mechanism for Urban-Scale Air Quality Simulation Models. ERT Inc., Newbury Park, CA and Statewide Air Pollution Research Center, University of California, Riverside, CA, 1987. Report to the US Environmental Protection Agency under contract 68-02-4104.
- Madronich S., 1987. Photodissociation in the atmosphere 1. Actinic flux and the effects of ground reflections and clouds. *J. Geophys. Res.* 92, 9740-9752.
- Madronich S., 2000. Atmospheric Chemistry Division, National Center for Atmospheric Research, Boulder, Colorado. Personal communication, April 2000.
- Meador W. E. and Weaver W. R., 1980. Two-stream approximations to radiative transfer in planetary atmospheres: A unified description of existing methods and a new improvement. *J. Atmos. Sci.* 37, 630-643.
- Meng Z., Dabdub D. and Seinfeld J. H., 1997. Chemical coupling between atmospheric ozone and particulate matter. *Science* 277, 116-119.
- Milford J. B., Gao D., Russell A. G. and McRae G. J., 1992. Use of sensitivity analysis to compare chemical mechanisms for air-quality modeling. *Environ. Sci. Technol.* 26, 1179-1189.
- Nakajima T. and Tanaka M., 1986. Matrix formulations for the transfer of solar radiation in a plane parallel scattering atmosphere. *J. Quant. Spectrosc. Radiat. Transfer.* 35, 13-21.
- NASA (2000). Total ozone mapping spectrometer (TOMS) ozone column retrievals. Goddard Space Flight Center, National Aeronautics and Space Administration. Downloaded from <http://toms.gsfc.nasa.gov/ozone/ozone01.html>.
- NOAA. United States Committee on Extension to the Standard Atmosphere. U.S. extension to the ICAO standard atmosphere. U.S. standard atmosphere, 1976. National Oceanic and Atmospheric Administration, U.S. Government Printing Office, Washington, D.C., 1976.
- Odum J. R., Jungkamp T. P. W., Griffin R. J., Flagan R. C. and Seinfeld J. H., 1997. The atmospheric aerosol-forming potential of whole gasoline vapor. *Science* 276, 96-99.
- Plass G. N., Kattawar G. W., Catchings F. E., 1973. Matrix operator theory of radiative transfer. 1: Rayleigh Scattering. *Appl. Opt.* 12, 314-329.

- Ruggaber A., Dlugi R. and Nakajima T., 1994. Modelling radiation quantities and photolysis frequencies in the troposphere. *J. Atmos. Chem.* 18, 171-210.
- Schmid B., Spyak P. R., Biggar S. F., Wehrli C., Sekler J., Ingold T., Mätzler C. and Kämpfer N., 1998. Evaluation of the applicability of solar and lamp radiometric calibrations of a precision Sun photometer operating between 300 and 1025 nm. *Appl. Opt.* 37, 3923-3941.
- Schmid B., Michalsky J., Halthorne R., Beauharnois M., Harrison L., Livingston J. and Russell P., 1999. Comparison of aerosol optical depth from four solar radiometers during the fall 1997 ARM intensive observation period. *J. Geophys. Res.* 17, 2725-2728.
- Schotland R. M. and Lea T. K., 1986. Bias in a solar constant determination by the Langley method due to structured atmospheric aerosol. *Appl. Opt.* 25, 2486-2491.
- Seinfeld J. H. and Pandis S. N. *Atmospheric Chemistry and Physics*. Wiley-Interscience, New York, NY, 1997.
- Shaw, G. E., Reagan, B. M. and Herman B. M., 1973. Investigations of atmospheric extinction using direct solar radiation measurements made with a multiple wavelength radiometer. *J. Appl. Meteor.* 12, 374-380.
- Shettle E. P. and Weinman J. A., 1970. The transfer of solar irradiance through inhomogeneous turbid atmospheres evaluated by Eddington's approximation. *J. Atmos. Sci.* 27, 1048-1055.
- Slusser J. R., Gibson J. H., Bigelow D. S., Kolinski D., Disterhoft D. P., Lantz K. and Beaubien A., 2000. Langley method of calibrating UV filter radiometers. *J. Geophys. Res.* 105, 4841-4849.
- Stamnes K. and Swanson R. A., 1981. A new look at the discrete-ordinate method for radiative transfer calculations in anisotropically scattering atmosphere. *J. Atmos. Sci.* 38, 387.
- Stamnes K., Tsay S.-C., Wiscombe W. and K. Jayaweera., 1988. Numerically stable algorithm for discrete-ordinate-method radiative transfer in multiple scattering and emitting layered media. *Appl. Opt.* 27, 2502-2509.
- Steele H. M. and Turco R. P., 1997. Separation of aerosol and gas components in the Halogen Occultation Experiment and the Stratospheric Aerosol and Gas Experiment (SAGE) II extinction measurements: Implications for SAGE II ozone concentrations and trends. *J. Geophys. Res.* 102, 19,665-19,681.

- Stephens G. L. Remote Sensing of the Lower Atmosphere. Oxford University Press, New York, NY, 1994.
- Taha H., 1998. Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, California. Personal communication, 1998.
- Thomason L. W., Herman B. M. and Reagan J. A., 1983. The effect of Atmospheric Attenuators with Structured Vertical Distributions on Air Mass Determinations and Langley Plot Analysis. *J. Atmos. Sci.* 40, 1851-1854.
- Tomasi C., Vitale V. and De Santis L. V., 1998. Relative optical mass functions for air, water vapour, ozone, and nitrogen dioxide in atmospheric models presenting different latitudinal and seasonal conditions. *Meteorol Atmos. Phys.* 65, 11-30.
- Toon O. B., McKay C. P., Ackerman T. P. and Santhanam K., 1989. Rapid calculation of radiative heating rates and photodissociation rates in inhomogeneous multiple scattering atmospheres. *J. Geophys. Res.* 94, 16,287-16,301.
- Vuilleumier L., Harley R. A. and Brown N. J., 1997. First- and Second-Order Sensitivity Analysis of a Photochemically Reactive System (a Green's Function Approach). *Environ. Sci. Technol.* 31, 1206-1217.
- Yang Y. J., Stockwell W. R. and Milford J. B., 1995. Uncertainties in incremental reactivities of volatile organic compounds. *Environ. Sci. Technol.* 29, 1336-1345.
- Yang Y. J., Stockwell W. R. and Milford J. B., 1996. Effect of chemical product yield uncertainties on reactivities of VOCs and emissions from reformulated gasolines and methanol fuels. *Environ. Sci. Technol.* 30, 1392-1397.