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A major area of scientific interest is in atmospheric photochemistry, in which the UV region is of prime importance. The absorption of O₂ and O₃ largely determine the extent of penetration of sunlight into the stratosphere and troposphere, where it causes photodissociation of a variety of molecules. The photodissociation of O₂ is especially important as the major source of odd oxygen.

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**THE AURIC-M
ATMOSPHERIC TRANSMISSION
AND RADIANCE MODEL**

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1.0 INTRODUCTION

The ultraviolet (UV) spectral region has current strong interest for both military and pure scientific studies. Military research, for example, often utilizes the UV emissions from rocket motor exhausts, and the possibility for smaller optical sensors than for the infrared (IR).¹ Wavelengths below 300 nm are important because atmospheric ozone and oxygen strongly attenuate the solar irradiance, leaving a dark background for target detection.

A major area of scientific interest is in atmospheric photochemistry, in which the UV region is of prime importance.^{2,3} The absorption of O₂ and O₃ largely determine the extent of penetration of sunlight into the stratosphere and troposphere, where it causes photodissociation of a variety of molecules. The photodissociation of O₂ is especially important as the major source of odd oxygen.³

The Air Force Phillips Laboratory, Geophysics Directorate, has long had a successful program for the development of computer models of atmospheric transmission and radiance, including the widely-distributed LOWTRAN and MODTRAN series.^{4,5} These models have strong capability in the infrared, and moderate capability in the visible and UV. The ongoing development of AURIC, the Atmospheric Ultraviolet Radiance Integrated Code, will provide a similar capability with specific attention to the UV.¹

One aspect of the AURIC development is the improvement of MODTRAN in the UV, resulting in a model called AURIC-M. This Fortran program extends MODTRAN both spectrally (out to 83,000 cm⁻¹, or 120 nm) and in altitude (up to 1000 km), and provides improved solar and O₂ absorption models. This report describes the development of AURIC-M, and provides instructions for its use. Section 2 contains the algorithmic and physical model descriptions, while Section 3 describes the changes in software usage from that of MODTRAN. The references are listed in Section 4, and a complete input description is given in Section 5.

2.0 TECHNICAL CHANGES

The AURIC-M model was developed from the existing MODTRAN model.⁵ Changes were made in a number of areas, including:

- 1) inclusion of better O₂ line and continuum absorption models from 40,600 cm⁻¹ to 66,000 cm⁻¹,
 - a) replacement of the older Schumann-Runge band model with a temperature-dependent model from 49,000 cm⁻¹ to 57,000 cm⁻¹ at 1 cm⁻¹ intervals,
 - b) replacement of the older Herzberg continuum model above 40,600 cm⁻¹ with a new Herzberg and Schumann-Runge combined continuum to 66,000 cm⁻¹,
- 2) increase in the number of atmospheric layers available for doing the calculations, easily changed with a re-compilation,
- 3) increase in the altitude extent of the atmospheric profile data for Model 6, the 1976 US Standard Atmosphere, to 1000 km, and
- 4) increase in the spectral extent and resolution of the solar irradiance model using 1987 SUSIM data.

These changes may all be accessed by a user via a simple flag in the first input card. The model may also be run with all of the new capabilities turned off, providing operation identical to that of MODTRAN or LOWTRAN7. The following sub-sections describe each AURIC modification.

2.1 Schumann-Runge Absorption Model

The Schumann-Runge (SR) bands of oxygen represent the major source of opacity in the important UV region from 175 to 200 nm,⁶ and are an important source of O₂ photodissociation.² Recent work by Minschwaner, et al,^{3,6} has provided an accurate SR absorption model at 0.5 cm⁻¹ resolution. A polynomial scheme was developed to approximate the temperature-dependence of the spectral cross-sections, with maximum errors of 15%.⁷ The algorithm expresses the cross-section as a quartic polynomial in temperature, with only the even terms non-zero. The spectral dependence resides entirely in the polynomial coefficients.

This formula allows the optical depth to be factored into spectrally-dependent and spectrally-independent factors. The spectral portion consists of the polynomial coefficients,

tabulated every 0.5 cm⁻¹ from 49,000 to 57,000 cm⁻¹. For accuracy, separate coefficients were developed for each of three temperature regions, from 130 to 190 k, 190 to 280 k, and 280 to 500 k. The spectrally-independent portion consists of only nine values, namely the atmospheric path column density, weighted by the temperature to the fourth, second, and zeroth powers, integrated separately in each of the three temperature ranges. Such temperature-weighted densities were previously incorporated into MODTRAN for the O₃ Hartley-Huggins band.

MODTRAN is designed to step spectrally in 1 cm⁻¹ increments, with the output optionally filtered to lower resolution. The molecular line absorption coefficients are stored at the necessary 1 cm⁻¹ resolution, while slowly-varying absorbers (e.g., molecular continua, aerosol extinctions) are accessed in 5 cm⁻¹ steps (usually with 20 cm⁻¹ resolution), and are interpolated to the 1 cm⁻¹ wavenumber grid.

For the Schumann-Runge model of Minschwaner, et al, a step of 0.5 cm⁻¹ is desired. However, major changes would be needed to modify the many MODTRAN routines from integer 1 cm⁻¹ steps to smaller floating-point steps. G. Anderson and A. Hall of the Phillips Laboratory investigated several methods of reducing the Schumann-Runge resolution to 1 cm⁻¹, and concluded that sufficient accuracy was achieved by simply sub-sampling the Minschwaner coefficients, taking every other one.⁷ A routine, "O2SRBD", was written to read in the Schumann-Runge spectral coefficients within the desired spectral range, and to return the values for any wavenumber.

The non-spectral portion of the model requires the path column density of O₂, scaled by the (normalized) temperature to the fourth, second, and zeroth powers, and stored separately for temperatures in each of three temperature ranges. The number of "species" was therefore increased by 9, and subroutine GEO was modified to compute and store the scaled column amounts.

Although the SR line absorption extends up to 57,000 cm⁻¹, the line wings form a quasi-continuum outside the band. The Minschwaner Model³ provides this contribution, which Minschwaner has fit to a quadratic polynomial in wavenumber, from 57,000 to 66,000 cm⁻¹.

2.2 Layering Increase

The need to add higher altitudes to the atmospheric profiles caused the need for an increase in the maximum number of layers in MODTRAN from the original 34. It was also known that this modification would provide benefits in other ways, and at all wavelengths, by allowing users to utilize more than 34 layers for other reasons. For example, long near-tangential paths are less

prone to errors in refraction and radiation transfer when the profile is finely layered. Having a larger dimension releases the user from having to tailor his profile, with many layers at some altitudes and very few layers elsewhere. Extra layers are also sometimes desired within and near inserted cloud decks.

There are, actually, several different types of layering within MODTRAN, although this is not obvious to the user. For example, there are "data layers", at which the profile is input or internally stored, and "calculation layers" (with parameters interpolated from the data layers) on which the computation is performed. This concept is a good one, as it allows for calculations to be made with many layers, where needed for accuracy, while keeping the input layers fixed.

The layering schemes currently implemented are:

- 1) The hard-coded data layering for Models 1 through 6, set in block data MLATBM with variable ALT, and passed in common block /MLATM/.
- 2) The hard-coded calculation layering for Models 1 through 6, set in subroutine FLAYZ with variables ZAER, ZNEW, and ZNEWV, and used locally to set the array ZMDL for use elsewhere in the program.
- 3) The user input data layers for Model 7, which become the calculation layers in that case.
- 4) Other specific data layering exists for clouds, rain rate, aerosol profile, and the Army Vertical Structure Algorithm, VSA. These are independent from the above layer types, and are inserted into the calculation layering as appropriate by routine FLAYZ.

At present, no independent user input calculation layering exists. This prevents the user from independently inputting data at given altitudes, while requesting the program to do the calculations at different (e.g. more) layers. By inputting only altitude data in Model 7 with the proper flags set, a user is able to run with Model 1 through 6 profiles, calculated at the input altitudes.

Increasing the "34 layer" dimension was a large task, since it was strongly embedded ("hardwired") within MODTRAN, along with its half, double, and triple (17, 68, and 102). Many variable dimensions, and loop limits, contained these values explicitly. In order to modify these, and to make future changes much easier, a Fortran PARAMETER "LAYDIM" was defined as the maximum number of layers for calculation, and was increased from 34 to 100. The multiples of 34 were replaced with other PARAMETERS, called LAYHAF, LAYTWO, and LAYTHR. All of these values were placed in a single file, called "AURIC.DEF", which is automatically inserted in

each required routine via the Fortran "INCLUDE" command. If a user needs to increase LAYDIM, he need only modify AURIC.DEF. and recompile the entire program. Although the INCLUDE command is not ANSI standard, it is available on nearly all modern compilers. On other compilers, an editor must be used to explicitly insert the file in place of the INCLUDE statement.

The Air Force desired to allow a user to run AURIC in a mode with all of the new options turned off, including the layering. For this reason, the original calculation layer altitudes were kept in place (array ZAER), and new ones were added in a separate variable (ZAUR), used only when the AURIC mode is on. The ZAER altitudes vary in 1 km steps from 0 to 25 km, in 5 km steps up through 50 km, with other layers at 70, 100, and 1000 km (34 altitudes). The new ZAUR altitudes vary in 1 km steps from 0 to 26 km, in 2 km steps up to 70 km, in 4 km steps up to 150 km, in 10 km steps up to 300 km, with other layers at 500, 750, and 1000 km (87 altitudes).

In MODTRAN, the default ZAER altitudes are modified if the user selects one of several different aerosol algorithms, including the VSA and cloud models. These options are also supported in AURIC mode, with the appropriate aerosol model altitudes replacing the ones in ZAUR.

2.3 Altitude Extension

MODTRAN contains six model atmosphere profiles within it, contained in block data MLATMB. There are 50 "data layer" altitudes defined (the number is now set in AURIC via the Fortran parameter MODDAT). These profiles step by 1 km from 0 to 25 km, by 2.5 km up to 50 km, and by 5 km up to 120 km. These data layers are still accessed when AURIC is run in MODTRAN mode.

Two new sets of data layers were added for AURIC, one for daytime (block data ALATMB) and one for nighttime (block data NLATMB). In the altitude regime from 0 to 50 km, the parameters were taken from the MODTRAN data set, but interpolated onto a different altitude grid. From 50 to 300 km, parameters from the SHARC model⁸ were used for Model 6, and zeros elsewhere. Above 300 km, values from the 1976 U.S. Standard Atmosphere were used for Model 6, and zeros elsewhere. A total of 104 layers were defined, with altitudes from 0 to 25 km by 1 km, up to 50 km by 2.5 km, up to 150 km by 2 km, up to 300 km by 10 km, with additional layers at 500, 750, and 1000 km. Models 1 through 5 were not filled out above 50 km because of the lack of appropriate SHARC and 1976 U.S. Standard data. In addition, the U.S. Standard Atmosphere lacks data above 300 km for all components except N₂, O₂, and the total air density.

2.4 Solar Irradiance Wavelength Extension

The extraterrestrial solar irradiance data stored within the model were extended to shorter wavelengths, using the 1987 SUSIM data taken from Spacelab2.⁹ The MODTRAN data extend up to 57,470 cm^{-1} . The new data extend from 25,003 to 82,987 cm^{-1} (120.5 to 399.95 nm) at 0.05 nm spacing, and with 0.15 nm spectral resolution. The new data are used above 25,000 cm^{-1} in AURIC mode. In MODTRAN mode, the original data set is used.

Since the SUSIM data are tabulated versus wavelength (nm), routine SUN was modified to access the appropriate data set, and to interpolate in wavelength where necessary.

3.0 MODEL USAGE CHANGES

Most of the changes from MODTRAN to AURIC were designed to not require any additional user input. A single input flag (described below) turns the AURIC mode on or off. Several new data files are required, but the user need not modify them.

Section 3.1 describes the AURIC input flag, and comments on the user restrictions in altitude profiles and spectral parameters. Section 3.2 describes the new data files.

3.1 Changes To The MODTRAN2 User Input

MODTRAN was designed to operate in two primary modes, either using the MODTRAN capabilities (higher spectral resolution and temperature-dependent band models), or defaulting to the operation of LOWTRAN7, the model on which MODTRAN was built. The run mode is controlled with a single input "flag" variable. While the MODTRAN mode is more accurate, it runs more slowly, and does not extend spectrally beyond 22,681 cm^{-1} (440 nm).

AURIC has similarly been designed with the user option for either LOWTRAN7, MODTRAN, or AURIC mode. The only user input change from MODTRAN is the substitution of a three-space character variable, "TYPROG", for the previous MODTRAN logical variable. MODTRAN is turned on, rather than LOWTRAN 7, if a "T" character is in the first space (for compatibility with MODTRAN). MODTRAN is also turned on if an "M" is in any of the three spaces. AURIC is turned on, independent of MODTRAN/LOWTRAN, if an "A" is in any of the three spaces. Since the upper atmosphere profile is day- and night-dependent, an "N" character in any of the three spaces will be used with AURIC to specify night. The characters "L" and "D"

may also be used to explicitly indicate LOWTRAN and "day" in the absence of "M" and "N". Note, however, that all of the above character flags must be upper case letters. The controlling Fortran statements in subroutine DRIVER are:

```
LOGICAL MODTRN,AURICL,NIGHT
CHARACTER*3 TYPROG
COMMON /PRGTYP/ AURICL,NIGHT
MODTRN=.FALSE.
AURICL=.FALSE.
NIGHT =.FALSE.
READ(IRD, '(A3,I2,12I5,F8.3,F7.2)') TYPROG,MODEL,ITYPE,IEMSCT,
& IMULT,M1,M2,M3,M4,M5,M6,MDEF,IM,NOPRT,TBOUND,SALB
IF(TYPROG(1:1).EQ.'T') MODTRN=.TRUE.
IF(TYPROG(1:1).EQ.'M') MODTRN=.TRUE.
IF(TYPROG(2:2).EQ.'M') MODTRN=.TRUE.
IF(TYPROG(3:3).EQ.'M') MODTRN=.TRUE.
IF(TYPROG(1:1).EQ.'A') AURICL=.TRUE.
IF(TYPROG(2:2).EQ.'A') AURICL=.TRUE.
IF(TYPROG(3:3).EQ.'A') AURICL=.TRUE.
IF(TYPROG(1:1).EQ.'N') NIGHT =.TRUE.
IF(TYPROG(2:2).EQ.'N') NIGHT =.TRUE.
IF(TYPROG(3:3).EQ.'N') NIGHT =.TRUE.
```

AURIC is delivered with the maximum number of calculational layers set to a value of LAYDIM = 100. This may be changed by editing the file AURIC.DEF, which gets included in the source code via the compiler. The other calculational parameters (e.g., LAYTWO) are defined via scaling LAYDIM, so the user need not modify them. The code must then be re-compiled for the re-dimensioning to take place.

The user may also wish to modify the default calculational layers (used except when Model=7), which are defined in array ZAUR within subroutine FLAYZ. These 87 layers are those used with atmospheric Models 1 through 6. If they are not modified, the user can only calculate with more layers by the use of Model 7. Runs with the six standard models will use the 87 calculation layers in ZAUR, plus any others called for by the user's selection of special aerosol options, including the Vertical Structure Algorithm (VSA) and cloud layers. These options can currently result in the use of up to 96 calculational layers.

Since the user-defined Model 7 allows all of the parameters (temperature, pressure, concentrations) to be interpolated from another model (e.g., from Model 6) via the variables M1 through M1 plus MDEF, the user may define a Model 7 input which specifies only the desired altitudes, and lets AURIC insert the proper parameters at each altitude. Note that when Model=7, the calculational layers are the same as the input data layers. If the default calculational layers in ZAUR are not changed, the user will always get the same ones when Models 1 through 6 are used.

MODTRAN is restricted to wavenumbers below 50,000 cm⁻¹ (wavelengths above 200 nm), and only the LOWTRAN7 mode is available from 22,681 to 50,000 cm⁻¹ (200 to 440 nm). In the LOWTRAN7 mode, the computations are made at 20 cm⁻¹ spectral resolution, in step sizes which are a multiple of 5 cm⁻¹. In the MODTRAN mode the computations are made internally in 1 cm⁻¹ steps, and are spectrally degraded to a user-specified resolution and step size. In the AURIC mode, the spectral step size is dependent on the spectral range, and on whether or not the MODTRAN flag was set. When the entire spectral range is in the UV region (above 25,000 cm⁻¹; below 400 nm) the internal step size is set to 1 cm⁻¹, and the output is degraded as requested by the user. When part of the spectral range is in the infrared or visible, the spectral resolution is set by the MODTRAN flag (i.e., 1 cm⁻¹ steps if MODTRAN is on, or a multiple of 5 cm⁻¹ if not.) The following table summarizes the utilization of various options versus the run mode. It shows some of the interplay between the MODTRAN and AURIC flags, coupled with the wavenumber restrictions on them.

3.2 Additional Data Files

Two types of fixed data files have been added to the model. Their formats are documented below.

3.2.1 Schumann-Runge Coefficient Files

Subroutine O2SRBD reads and returns the polynomial coefficients for the O₂ Schumann-Runge band, A, B, and C. Absorption cross sections are computed from these, and the temperature, by:

$$\text{Cross section (cm}^2\text{)} = (A \cdot X^2 + B \cdot X + C) \cdot 10^{-20},$$

where,

$$X = [(100-T)/10]^2,$$

Status of AURIC Layering and Spectral Options Versus Run Mode

Mode Name	MODTRAN Flag On?	AURIC Flag On?	Starting Wavenumber (cm ⁻¹)	Ending Wavenumber ^a (cm ⁻¹)	Internal Step Size (cm ⁻¹)	Maximum # of Layers
LOWTRAN7	N	N	$\omega_1 < \omega_2$	any	N*5 ^b	34
MODTRAN	Y	N	$\omega_1 < \omega_2$	$\omega_2 < 22,681$	1	34
LOWTRAN7 ^c	Y	N	$\omega_1 < \omega_2$	$\omega_2 \geq 22,681$	N*5 ^c	34
AURIC/IR-Vis	N	Y	$\omega_1 < 25,000$	$\omega_1 < \omega_2$	N*5	100
AURIC/UV	N	Y	$\omega_1 \geq 25,000$	$\omega_1 < \omega_2$	1 ^d	100
AUR/MOD/IR-Vis	Y	Y	$\omega_1 < \omega_2$	$\omega_2 < 22,681$	1	100
AUR/LOW	Y	Y	$\omega_1 < 25,000$	$\omega_2 \geq 22,681$	N*5	100
AURIC/UV	Y	Y	$\omega_1 \geq 25,000$	$\omega_1 < \omega_2$	1 ^d	100

a All wavenumbers must be less than 83,000

b Means any positive integer multiple of 5

c Beyond band model data; MODTRAN mode is turned off internally

d For Schumann-Runge Model

and T is the temperature in Kelvins. Each coefficient is tabulated over the wavenumber range from 49,001 to 57,000 cm⁻¹, at intervals of 1 cm⁻¹, and over the three temperature ranges: 130K to 190K, 190K to 280K, and 280K to 500K. The three files 130190.COF, 190280.COF, and 280500.COF are read the first time through; those coefficients within the user's spectral range are stored.

Each file begins with three header lines, which are not used by AURIC. A list of wavenumbers, and coefficients for each, is read next. The file format is:

<u>Line Type #</u>	<u>Format</u>	<u>Variables</u>	<u>Type</u>	<u>Definition</u>
LINE TYPE 1	A80	LINE	CHAR*80	- not used -
- Repeat line type 1 for a total of three lines -				
LINE TYPE 2	F8.1,3E11.3,F6.2,F8.1	WN	REAL	Wavenumber (cm ⁻¹)
		TCA	REAL	Coefficient A
		TCB	REAL	Coefficient B
		TCC	REAL	Coefficient C
		DUMP1	REAL	- not used -
		DUMP2	REAL	- not used -

- Repeat line type 2 for a total of 8000 lines -

3.2.2 SUSIM Solar Irradiance Data

Subroutine RDSUSM reads the data file 'IRRAD_HI.INP', containing the high-resolution SUSIM solar irradiance data. This data set covers the spectral range from 120.5 to 399.95 nm in steps of 0.05 nm (5590 values). The original data file had the irradiances stored 10 per line, with a wavelength beginning each line. Each of the original lines has been divided into two, so that each line is now less than 80 characters wide, for easy portability. The first line has the wavelength and six irradiance values, followed by the other four values on the next line. The format is:

<u>Line Type #</u>	<u>Format</u>	<u>Variables</u>	<u>Type</u>	<u>Definition</u>
LINE TYPE 1	1X,F6.2,6E12.4	LAMBDA	REAL	Wavelength (nm) [not used]
		IRRAD(J)	REAL	Irradiance at LAMBDA
		IRRAD(J+1)	REAL	Irradiance at LAMBDA + 0.05nm
		⋮		
		IRRAD(J+5)	REAL	Irradiance at LAMBDA + 0.25nm
LINE TYPE 2	E11.4,3E12.4	IRRAD(J+6)	REAL	Irradiance at LAMBDA + 0.30nm
		⋮		
		IRRAD(J+9)	REAL	Irradiance at LAMBDA + 0.45nm

- Repeat the above pair of lines a total of 559 times -

This format produces a file with 1,118 lines (559 line pairs).

4.0 REFERENCES

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5.0 USER INSTRUCTIONS

[--> Will insert MODTRAN2 user instructions, to be provided by
PL, and modified for AURIC <--]