GENLN3: A General Line-by-Line Atmospheric Transmittance and Radiance Model

Version 1.0
Description and Users Guide

Gene L. Francis
David P. Edwards
Thomas Heinemann
The Technical Notes series provides an outlet for a variety of NCAR Manuscripts that contribute in specialized ways to the body of scientific knowledge but that are not yet at a point of a formal journal, monograph or book publication. Reports in this series are issued by the NCAR scientific divisions, serviced by OpenSky and operated through the NCAR Library. Designation symbols for the series include:

**EDD – Engineering, Design, or Development Reports**
Equipment descriptions, test results, instrumentation, and operating and maintenance manuals.

**IA – Instructional Aids**
Instruction manuals, bibliographies, film supplements, and other research or instructional aids.

**PPR – Program Progress Reports**
Field program reports, interim and working reports, survey reports, and plans for experiments.

**PROC – Proceedings**
Documentation or symposia, colloquia, conferences, workshops, and lectures. (Distribution maybe limited to attendees).

**STR – Scientific and Technical Reports**
Data compilations, theoretical and numerical investigations, and experimental results.

The National Center for Atmospheric Research (NCAR) is operated by the nonprofit University Corporation for Atmospheric Research (UCAR) under the sponsorship of the National Science Foundation. Any opinions, findings, conclusions, or recommendations expressed in this publication are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

National Center for Atmospheric Research  
P. O. Box 3000  
Boulder, Colorado 80307-3000
GENLN3: A General Line-by-Line Atmospheric Transmittance and Radiance Model

Version 1.0:
Description and Users Guide

Gene L. Francis
National Center for Atmospheric Research (NCAR)

David P. Edwards
National Center for Atmospheric Research (NCAR)

Thomas Heinemann
European Organisation for the Exploitation of Meteorological Satellites (EUMETSAT)
How to Cite this Document:

doi:10.5065/ccfx-te27
GENLN3: A General Line-by-Line Atmospheric Transmittance and Radiance Model

Version 1.0
Description and Users Guide

G. L. Francis, D. P. Edwards, T. Heinemann

Atmospheric Chemistry Observations and Modeling (ACOM) Laboratory
National Center for Atmospheric Research
Boulder, CO USA
# Contents

1 Preface to GENLN3 Version 1.0  
2 Preface to GENLN2 Version 3.0  
3 Acknowledgements  
4 Introduction  
   4.1 Atmospheric Radiative Transfer  
   4.2 The GENLN3 Suite of Programs  
   4.3 GENLN3 Input File Formats and Processing Conventions  
      4.3.1 Input File Syntax  
      4.3.2 Processing Conventions  
      4.3.3 GENLN3 Implementation  
5 Spectral Line Data: Program HITRUN  
   5.1 Spectral Line Database  
   5.2 Overview of Program HITRUN  
   5.3 Description of the HITRUN Input File  
6 Atmospheric Modeling  
   6.1 Layers, Paths, and Mixed Paths  
   6.2 Atmospheric Profiles  
   6.3 Atmospheric Layering  
7 The Line-by-Line Calculation: Program GENRUN  
   7.1 Overview  
   7.2 Spectral Modeling  
   7.3 Line Shape Modeling  
   7.4 Continuum Absorption  
      7.4.1 H\textsubscript{2}O  
      7.4.2 CO\textsubscript{2}, O\textsubscript{2}, N\textsubscript{2}  
   7.5 Molecular Cross-Section Data  
   7.6 Aerosol Model  
   7.7 The Line-By-Line Calculation  
   7.8 Transmittance Calculations  
   7.9 Radiance Calculations  
   7.10 Description of the GENRUN Input File  
8 Example Calculations  
   8.1 Example 1: Nadir calculation using the NADIR keyword  
      8.1.1 Example 1: HITRUN Input File  
      8.1.2 Example 1: GENRUN Input File  
      8.1.3 Example 1: Output  
   8.2 Example 2: Nadir calculation using the PATH keyword  
      8.2.1 Example 2: HITRUN Input File  
      8.2.2 Example 2: GENRUN Input File  
      8.2.3 Example 2: Output  
   8.3 Example 3: Limb calculation using the LIMB keyword  
      8.3.1 Example 3: HITRUN Input File  
      8.3.2 Example 3: GENRUN Input File  
      8.3.3 Example 3: Output
8.4 Example 4: Limb calculation using the PATH keyword ........................................... 59
8.4.1 Example 4: HITRUN Input File ................................................................. 59
8.4.2 Example 4: GENRUN Input File ................................................................. 59
8.4.3 Example 4: Output ....................................................................................... 63
8.5 Example 5: Gas cell transmittance calculation using the CELL keyword .............. 64
8.5.1 Example 5: HITRUN Input File ................................................................. 64
8.5.2 Example 5: GENRUN Input File ................................................................. 65
8.5.3 Example 5: Input file ct.path .................................................................... 66
8.5.4 Example 5: Output ....................................................................................... 66
8.6 Example 6: Flux calculation using the FLUX keyword ........................................ 66
8.6.1 Example 6: HITRUN Input File ................................................................. 67
8.6.2 Example 6: GENRUN Input File ................................................................. 67
8.6.3 Example 6: Output ....................................................................................... 70
8.7 Example 7: Radiance looking upward through atmosphere to space .................. 71
8.7.1 Example 7: HITRUN Input File ................................................................. 71
8.7.2 Example 7: GENRUN Input File ................................................................. 71
8.7.3 Example 7: Output ....................................................................................... 74
8.8 Example 8: NADIR calculation which includes sulfate aerosol ......................... 74
8.8.1 Example 8: HITRUN Input File ................................................................. 75
8.8.2 Example 8: GENRUN Input File ................................................................. 75
8.8.3 Example 8: Output ....................................................................................... 79

References ............................................................................................................... 79
List of Figures

1. Decomposition of an atmospheric path of mixed gases into layers and single gas paths. 15
2. Geometry of a limb path through a refractive atmosphere. 17
3. The GENLN3 spectral calculation scheme. 25
4. Illustration of mixed paths formed from the paths of Figure 1 and defined by the mixing table above. 28
5. Example of profile data set required with keyword USER_PROFILE. 32
6. Example 1 (Nadir calculation via NADIR keyword): Individual transmittance spectra for H$_2$O, CO$_2$, O$_3$, and CFC12. Also the total transmittance of all gases calculated two ways, and their (small) difference. 44
7. Example 1 (Nadir calculation via NADIR keyword): TOA total nadir radiance due to H$_2$O, CO$_2$, O$_3$, and CFC12 along with solar, surface, and atmospheric contributions. Verification that the sum of the radiance components is equal to the independently-reported total radiance. Nadir radiance spectra from TOA down to selected levels. 45
8. Example 1 (Nadir calculation via NADIR keyword): TOA radiance contributions by H$_2$O, CO$_2$, O$_3$, and CFC12 individually. Also, the total radiance calculated two ways, and their (small) difference. 46
9. Example 2 (Nadir calculation via PATH keyword): Individual TOA transmittance spectra for H$_2$O, CO$_2$, O$_3$, and CFC12 computed using PATH (first column) and comparison with spectra obtained using NADIR (second column). Differences between the two calculations (third column) are small. 51
10. Example 2 (Nadir calculation via PATH keyword): TOA radiance spectra due to H$_2$O, CO$_2$, O$_3$, and CFC12 for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated and plotted on the fine mesh grid. 52
11. Example 2 (Nadir calculation via PATH keyword): TOA radiance spectra due to H$_2$O, CO$_2$, O$_3$, and CFC12 for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated on the fine mesh but plotted on the wide mesh integrated grid. 53
12. Example 2 (Nadir calculation via PATH keyword): TOA transmittance spectra due to H$_2$O, CO$_2$, O$_3$, and CFC12 for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated on the fine mesh but plotted on the wide mesh integrated grid. 54
13. Example 2 (Nadir calculation via PATH keyword): TOA transmittance spectra due to H$_2$O, CO$_2$, O$_3$, and CFC12 for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated on the fine mesh but plotted on the wide mesh integrated grid. 55
14. Example 3 (Limb calculation via LIMB keyword): Total limb radiance and individual contributions by CO$_2$ and O$_3$ for a 30km tangent height. Total limb transmittance and individual contributions by CO$_2$ and O$_3$. Limb transmittance for levels 30, 20, 10, and 0, the latter lying near TOA. Transmittance and radiance differences for two calculation techniques are small. 59
15. Example 4 (Limb calculation via PATH keyword): Total limb transmittance due to CO$_2$ and O$_3$ for a 30 km tangent height computed using PATH, and comparison with transmittance obtained using LIMB. 63
16. Example 4 (Limb calculation via PATH keyword): Individual limb radiance contributions from CO$_2$ and O$_3$ for a 30 km tangent height. 64
Example 5 (Cell transmittance via CELL keyword): Segment of the Average and Difference transmittance spectra for a two-state model of a pressure-modulated radiometer (PMR). The spectral interval plotted lies in the 0–1 $CO$ fundamental band. Cell calculations similar to these enable global remote sensing of tropospheric $CO$ via gas correlation radiometry by the NASA EOS/MOPITT instrument onboard the Terra spacecraft [Drummond et al., 2010].

Example 6 (Flux calculation via FLUX keyword): Upward, downward, and total flux as a function of altitude, together with the corresponding cooling rate, for the infrared wavenumber interval [980, 1180], which includes the strong 9.6 $\mu m$ $O_3$ band. Gases used in this calculation are $H_2O$, $CO_2$, $O_3$, and $CFC12$.

Example 7 (Radiance looking upward through atmosphere to space): Emission spectra between selected atmospheric levels and TOA. The atmosphere contains $H_2O$, $CO_2$, $O_3$, and $CFC12$. The bottom plot is the spectrum measured at the surface.

Example 8 (NADIR calculation incorporating sulfate aerosol): Individual transmittance spectra for $H_2O$, $CO_2$, $O_3$, $H_2SO_4$, and $CFC12$. Also the total transmittance of all gases calculated two ways, and their (small) difference.
1 Preface to GENLN3 Version 1.0

In 1991 the line-by-line code GENLN2 Version 3.0 was released to the scientific community. In the intervening years it has been widely applied to interests as diverse as satellite remote sensing of the earth and planets, laboratory radiative transfer modeling, and earth-system climate science. The preface to the original GENLN2 NCAR Technical Note included below gives further information on the model’s origin, design philosophy, and early development.

In response to rapid advances in computer technology, together with an expanding GENLN2 user community, interest developed in updating the code to take advantage of modern programming practices and data formats within a user-friendly setting. The result, GENLN3 Version 1.0, is described in this document. Although GENLN3 has been available from NCAR for some time, a formal description has hitherto been lacking. That deficiency is addressed with this publication. Users already familiar with GENLN2 will find that GENLN3 provides a familiar work environment while offering simplifications and additional options. We believe that GENLN3, building on the success of earlier versions, will continue to be an important research tool in the years ahead. Requests for the GENLN3 software distribution may be communicated to GLF or DPE at the email addresses given below. We also welcome all comments and suggestions.

Gene L. Francis (gfrancis@ucar.edu)
David P. Edwards (edwards@ucar.edu)
Thomas Heinemann (Thomas.Heinemann@eumetsat.int)

Atmospheric Chemistry Observations and Modeling (ACOM) Laboratory
National Center for Atmospheric Research
Boulder, Colorado USA
November 2023

Document version 15:36 11/10/2023
2 Preface to GENLN2 Version 3.0

This report constitutes the latest documentation for Version 3.0 of the GENLN2 suite of programs as of November 1991. The need for a new atmospheric transmittance and radiance model at Oxford was recognized by John Eyre of the UK Meteorological Office Unit in the Robert Hooke Institute for Cooperative Atmospheric Research in 1986. At the time, more than 25 members of the Department of Atmospheric Physics and Hooke Institute at Oxford University were engaged in radiative transfer calculations or were direct users of such data. It was decided that there was a strong case for developing a general purpose computation facility which would reduce the time spent duplicating effort in this area. Previously, a general line-by-line code GENLIN had been in use in Oxford. This along with other local codes was found to be limiting and inflexible, and although powerful facilities already existed, for example the Air Force Geophysical Laboratory’s FASCODE a total re-design to meet current and anticipated needs was considered justified. This would hopefully promote understanding of the physical method and avoid the “black-box” approach to computer modeling. The essential computational model was designed first and coded afterwards. The main aims were efficiency of calculation and a clear modular structure so that the model can be easily adapted as a research tool for specific needs. This has taken precedence over speed of computation or losing sight of the physics in difficult-to-understand algorithms. The model can then be used in an educational role and enables workers to refine the treatment of one part of the problem in isolation. Conversely, computations may also be performed quickly and without the users having detailed knowledge of the calculation methods involved. This report is intended to be a working document for those using GENLN2. A separate section is devoted to each of the programs that comprise the GENLN2 suite. Each section begins with a brief overview of the purpose of the program and the physics involved. This is followed by a detailed description of the code structure, required input and code implementation. The appendices include the input and output for two example calculations. Part of the work presented here was done during the time I held a post-doctoral position in the Satellite Meteorology Group of the Hooke Institute in Oxford. The project has continued since I moved to the Global Atmospheric Change Section of the Atmospheric Chemistry Division at the National Center for Atmospheric Research, Boulder CO.

David P. Edwards
Atmospheric Chemistry Division
National Center for Atmospheric Research Boulder, CO
November 1991
3 Acknowledgements

We are grateful to the following colleagues for their interest in GENLN3 and their use of the code. Through their help we have identified and corrected errors, added new options of community interest, clarified the software structure, and improved the initially meager GENLN3 documentation. Our thanks to all: William Collins, Tilak Hewegama, Alyn Lambert, Steve Massie, Jörn Unger mann, and Geronimo Villanueva.

We appreciate and acknowledge use of the HITRAN spectral database. GENLN3 users are asked to provide proper citation and description when presenting work based on HITRAN. A complete statement of requirements by the HITRAN team accompanies the HITRAN distribution.

In the example calculations GENLN3 output is plotted using IDL (Interactive Data Language), a product of NV5 Geospatial.

GENLN3 uses netCDF software developed by UCAR/Unidata.
4 Introduction

4.1 Atmospheric Radiative Transfer

Many workers in atmospheric physics and related fields are involved in transmittance and radiance calculations or are direct users of this information. The applications are varied, ranging through remote sensing and satellite meteorology, the measurement of atmospheric constituent gases, comparison calculations with laboratory spectroscopy studies, and developing radiation schemes as a basis for climate models. Calculations are performed over large spectral ranges, from the visible to the microwave, and many radiating gases and atmospheric trace constituents are considered. The physics that must be included has resulted in large and complex computer models. GENLN3 is a general purpose line-by-line model updating and extending its predecessor GENLN2 [Edwards, 1992].

Although there is great diversity in these calculations, at the heart of each lies an analysis of the effect of absorbing and emitting gases on the propagation of electromagnetic radiation. The computational modeling requirements for widely differing cases have much in common and general purpose radiative transfer models have been developed. For calculations where the detailed spectral structure is important a high resolution method is necessary. This takes a line-by-line approach where the absorption and emission of radiation by each molecular transition is considered in turn over the spectral range of interest.

Throughout this document we use the mixed-units conventions followed in the HITRAN database [Rothman et al., 2013].

Consider radiation of wavenumber $\nu$ [cm$^{-1}$] passing in the $z$-direction through an element of absorber thickness $dz$ [cm]. The radiation attenuation is

$$dI(\nu, z) = -I(\nu, z)k(\nu, z)\rho_a(z)dz,$$

(1)

where $I(\nu, z)$ is the radiation intensity [W/(m$^2$.sr.cm$^{-1}$)], $\rho_a(z)$ is the absorber number density [molecules.cm$^{-3}$], and $k(\nu, z)$ is the monochromatic absorption coefficient (also termed the cross-section) [1/(molecules.cm$^{-2}$)].

Integrating this equation from a source point $z_s$ to an observation point $z_{\text{obs}}$ gives

$$\int_{I(\nu, z_s)}^{I(\nu, z_{\text{obs}})} dI(\nu, z) = \int_{z_s}^{z_{\text{obs}}} k(\nu, z)\rho_a(z)dz,$$

(2)

and performing the integral

$$\tau(\nu, z_s, z_{\text{obs}}) = \frac{I(\nu, z_{\text{obs}})}{I(\nu, z_s)} = \exp\left(-\int_{z_s}^{z_{\text{obs}}} k(\nu, z)\rho_a(z)dz\right),$$

(3)

where $\tau(\nu, z_s, z_{\text{obs}})$ is defined as the transmittance between $z_s$ and $z_{\text{obs}}$.

The element of absorbing gas will also emit radiation whose intensity depends on its temperature $T$ [K]. If the element were enclosed in a perfectly black box, then the radiation intensity $B(\nu, T)$ [W/(m$^2$.sr.cm$^{-1}$)] entering the gas would be given by the Planck function

$$B(\nu, T) = \frac{c_1\nu^3}{\exp(c_2\nu/T) - 1},$$

(4)

where $c_1 = 2hc^2 = 1.1911 \times 10^{-8}$ [W/(m$^2$.sr.cm$^{-1}$)], $c_2 = hc/k = 1.439$ [K/cm$^{-1}$], and $h$, $k$, and $c$ are respectively Planck’s constant, Boltzmann’s constant, and the speed of light. Thus from Equation [1] the absorbed radiation in the $z$-direction would be $B(\nu, T)k(\nu, z)\rho_a(z)dz$. Assuming the gas is in local thermodynamic equilibrium, the temperature must remain constant and it follows from Kirchhoff’s law that the radiation intensity emitted in the $z$-direction will also be

$$B(\nu, T)k(\nu, z)\rho_a(z)dz,$$

(5)
The total radiative transfer equation will therefore have two parts: a transmitted radiation component which depends on the intensity at $z_s$ and the transmittance from $z_s$ to $z_{obs}$, and a radiation component due to the emission from all elements $dz$ between $z_s$ and $z_{obs}$ that actually arrive at $z_{obs}$,

$$I(\nu, z_{obs}) = I(\nu, z_s)\tau(\nu, z_s, z_{obs}) + \int_{z_s}^{z_{obs}} B(\nu, T(z))k(\nu, z)\rho_a(z)\tau(\nu, z, z_{obs})dz. \quad (6)$$

Solving this radiative transfer equation for the atmosphere is the basic aim of the GENLN3 code.

### 4.2 The GENLN3 Suite of Programs

GENLN3 consists of two executable codes, HITRUN and GENRUN. The input file for HITRUN is named `hitrun_input`. The input file for GENRUN is named `genln3_input`. To compile all of GENLN3, type “gmakeall” (one word, no quotes). This is a simple csh script that calls `gmake` two times to successively create HITRUN and GENRUN.

**HITRUN**

Program HITRUN creates the binary spectral line data file used by GENRUN. The inputs to HITRUN are 1) the user input file `hitrun_input` defining the calculation, and 2) one or more line data files in HITRAN format. The output is the GENRUN line data file in F90 binary format. The output file name is user-specified.

**GENRUN**

Program GENRUN performs the line-by-line calculation. It is based on specified profiles of temperature, pressure, density, and gas mixing ratio. The geometry of the calculation is assigned to compute path data as needed. A path is the basic unit for calculation of optical depth in GENRUN. After layering, a ray path is defined within each layer. GENRUN contains all the functionality of the former GENLN2 LAYERS program. Folding the GENLN2 LAYERS calculation into GENLN3 simplifies the code use.

Inputs for GENRUN are 1) the F90 binary line data file from HITRUN providing the spectral parameters, and 2) the user input file `genln3_input` defining the calculation. GENRUN produces two output files. One is a formatted ASCII file (`genln3_ascii_summary.out`) which contains a summary of both the user input and calculation output. The second output file is used with the post-processing programs. It is written in NetCDF and contains all specified output, in particular the spectra. Its name is user-specified.

The GENLN3 distribution has eliminated all the post-processing programs formerly included in GENLN2, specifically `GENGRP`, `RDOUT`, `BRIGHT`, and `RADTEM`. GENLN3 has adopted the viewpoint that post-processing tasks (e.g., filtering, integrating, subsetting, FFT) can be readily performed by the user with any software package that reads NetCDF. In the examples discussed in this document, the GENLN3 NetCDF output is read and displayed using IDL.

The NetCDF output file also includes a copy of the input file read by GENRUN. In this way the output file is clearly tied to the input file used to create it.

Overall GENLN3 is backwards-compatible with the functionality provided by GENLN2.

### 4.3 GENLN3 Input File Formats and Processing Conventions

GENLN3 uses an input file syntax different from GENLN2. Detailed descriptions of the HITRUN and GENRUN input files, and various file options, are given in Section 5.3 and Section 7.10. Below is a nine-point summary of the conventions and rules governing the overall input file structure.
4.3.1 Input File Syntax

1) GENLN3 input files consist of “blocks” and “keywords”.
2) Lines that begin with an asterisk (*) define “blocks”. Blocks provide overall organization of the input information.
3) Lines that begin with a dollar sign ($) define “keywords”. Keywords occur within blocks.
4) Lines beginning with an exclamation point (!) are ignored. Blank lines are ignored.
5) Blocks or keyword lines beginning with “!” are ignored, together with all the associated data. This avoids having to repeatedly type many “!” symbols for lists of associated data.
6) Strings between colons are comments : this is a comment :
7) There is no required ordering of blocks. That is, blocks may appear in arbitrary order.
8) When a keyword has been read by HITRUN or GENRUN, the program expects certain relevant parameters to follow. Some input sections are mandatory and are required to set up the basic problem. In other cases, there may be a choice of parameters depending on the required calculation. For example, MODE is a keyword which can take the “keyword values” NADIR, LIMB, PATH, CELL, and FLUX.
9) For simplicity, in this document we avoid the pedantic distinction between keywords and their possible values. We will casually refer to keywords and keyword values with the same term (e.g. the “NADIR keyword” rather than the “NADIR keyword value”).

To gain experience, run GENLN3 with different keywords turned on and off. Try various combinations of keywords within blocks. The code will attempt to exit smoothly and provide user-friendly diagnostics if certain combinations are not permitted.

4.3.2 Processing Conventions

1) Solar Radiance: The downwelling solar radiance contribution is included in GENLN3 radiance calculations, unless the MODE is CELL or PATH. A solar contribution is not included in CELL calculations because CELL calculations only produce transmittance spectra, not radiances. The solar contribution is NOT included in PATH calculations to maintain backwards compatibility with GENLN2 conventions. This solar radiance contribution may be turned on or off by changing the variable SUN_TEMP in subroutine globals_mod.f90 to a value other than 5777, then recompiling. If the user is not doing a CELL calculation, a comment is printed in the GENLN3 ASCII output file genln3_ascii_summary.out stating whether the solar radiance is, or is not, included.

2) Solar Transmittance Spectrum: The downwelling solar radiance at the top-of-atmosphere is treated as a Planck blackbody. No solar transmittance spectra is included to account, for example, for the absorption of the solar chromosphere. If the user wants to modify the solar calculation to include a user-specified solar transmittance, the calculation of array fluxstoa in subroutine emission.f90 needs to be multiplied pointwise by the transmittance spectra.

3) Code Optimization: Like any complex software, GENLN3 should first be compiled and tested using little or no compiler optimization. This may run slowly, but it is a prudent way to start. When recompiled at higher optimization one should check for any anomalous behavior due to the compiler rearranging code, etc. If anomalous behavior occurs at high optimization, then return to a lower level. These are common software concerns and not a problem with GENLN3 itself.

4.3.3 GENLN3 Implementation

GENLN3 is written in FORTRAN 90. The module globals_mod.f90 assigns both the numerical KIND and the HITRUN unformatted output file record length. These can easily be changed to accommodate specific compiler and hardware requirements. The module setup_mod.f90 assigns the floating point precision NUM_DIGITS_HP and the record length MACHINE_TYPE. To extend the functionality of
FORTRAN 90 and provide more GENLN3 flexibility, a collection of routines were written to allocate, deallocate, and reallocate arrays at run time. These are defined in tools_mod.f90. These routines are a significant code simplification, and completely eliminate the tedious specification of array sizes and repeated recompilation found in GENLN2. The Makefile is intended as a working guide and compiles GENLN3 successfully on local NCAR platforms; minor modifications will permit its use on other systems.

5 Spectral Line Data: Program HITRUN

5.1 Spectral Line Database

The increasing use of line-by-line radiative transfer codes has been made possible by the availability of comprehensive molecular spectral line data compilations. These draw on the laboratory and atmospheric measurements and calculations of many workers and are periodically updated.

GENLN3 uses the HITRAN database. The 2012 edition [Rothman et al., 2013] is currently provided with the GENLN3 software. HITRAN is updated in the GENLN3 software at irregular intervals. HITRAN 2012 contains line parameters for 47 molecules in ASCII format and molecular cross section data sets for 38 molecules. GENLN3 (like GENLN2) allows the user to override portions of the default HITRAN distribution by specifying a user-supplied source of HITRAN data in the HITRUN input file (Section 5.2 below). Section 7 contains a detailed description of how HITRAN is implemented in GENLN3. Note that HITRAN line strengths for a particular isotope are weighted according to the naturally occurring terrestrial abundance of the isotope. Therefore, in general these will need to be modified if applied to non-terrestrial settings.

5.2 Overview of Program HITRUN

The program HITRUN has the facility for merging several line data bases to form a single line file that is then used by GENRUN. This is useful for updating lines on the HITRAN database with new line data as it becomes available. The input to the program is a user-supplied input file described in Section 5.3, together with one or more HITRAN line databases.

The HITRAN database, as distributed, is blocked with numerous lines per record. HITRUN modifies this format so that each line occupies one record.

1. Line records from the input line data bases are first merged together in order of increasing wavenumber between the lower and upper wavenumber bounds specified by the user in the HITRUN input. A direct access, unformatted output line file is created and the following stages manipulate this new output file. The option of creating a sub-set of the HITRAN data base will be useful for users with limited on-line storage who are only interested in part of the spectrum.

2. To avoid possible computer underflow problems or very small numbers being set equal to zero, HITRUN scales up the value of the line strength, originally in units of $cm^{-1}/(molecule.cm^{-2})$, by the Avogadro number ($6.022 \times 10^{26}$ molecules/kmole). The line strength then has units of $cm^{-1}/(kmole.cm^{-2})$. In the GENLN3 input file, the gas amounts are stated in units of kmole.cm$^{-2}$ to compensate for this scaling.

3. Each line record is assigned a status number according to which input data base the line came from. These status numbers are defined by the user in the HITRUN input file. If there is more than one input data base and new line data is merged with older data, there may be duplicate lines. These will be distinguished by having different status numbers.

4. Each line record is assigned a forward pointer. This indicates how many lines forward of the current record the next line record occurs for the same gas. This allows lines for any particular gas or set of gases to be accessed directly without reading unwanted line records. This results in a
considerable time saving over reading and sorting all lines sequentially during the execution of the GENL3 line-by-line program.

5. Every 200 line records a forward pointer block is inserted into the line file. This block comprises 3 records that contain the forward pointers to each of the gases on the line file. It ensures that no more than 200 line records will ever be read by GENL3 in searching for the first occurrence of a line for a particular wanted gas.

6. By comparing the quantum numbers of the line transitions, a check is made for duplicate lines on the output line file. The duplicate lines with the lower status number are flagged by changing the status number to the negative of itself. The input to GENL3 allows the user to choose which status lines are used in the line-by-line calculation.

5.3 Description of the HITRUN Input File

*TITLES
This block is mandatory.
$ TITLE is the title of the HITRUN run. This is used as a header for the output line file and should be descriptive.

*LINDAT
This block is mandatory.
$ NUMBER_OF_FILES (integer) - The number of line data base files having the HITRAN format that will be merged to form the unformatted direct access output line file read by GENRUN.
$ FILE_TABLE - Precedes the list of HITRAN format data files. Each line in the list consists of a file “status number” (integer), followed by a comma, followed by the ASCII file name (string).

When a new line data base is merged with the HITRAN data base, some lines that have been up-dated may be duplicated. When HITRUN encounters duplicate lines for a given transition, those with the higher status number assume priority. Status numbers should therefore be assigned with new up-dates having higher values. The HITRAN data base will always have the lowest status number and this should be set equal to 10. It is possible to select which version of duplicate lines are used by the GENL3 line-by-line calculation. This will be described in full in Section 7.10 but for clarity will be mentioned here. A GENL3 status parameter $ichose is assigned to each gas. This specifies that for the gas in question and for any given transition, the line version with the highest status will be used by GENL3 up to and including a line with status $ichose.

*RANGES
This block is mandatory.
$ LOWER_WN (real) - The lower wavenumber boundary for selecting lines from the input data bases.
$ UPPER_WN (real) - The upper wavenumber boundary for selecting lines from the input data bases.

These two parameters allow a subset of the entire HITRAN data base to be created.

*HITOUT
This block is mandatory.
$ HITLIN_OUTPUT_FILE (string) - The file name of the merged, unformatted direct access output line file that will be used by GENRUN.

*ENDINP
This block is mandatory. It marks the end of the input file.
6 Atmospheric Modeling

6.1 Layers, Paths, and Mixed Paths

The concepts of layers, paths and mixed paths are important for understanding the GENLN3 calculation procedure. These quantities are defined below and used in the following discussions.

Layers

The inhomogeneous nature of the atmosphere along a radiation path is most readily treated by sub-dividing the atmosphere into a set of layers. In this way the integration over \( z \) in Eqn 6 becomes a summation over the constituent layers. The layer boundaries should be chosen so the gas in the layer may be considered homogeneous and well represented by appropriate Curtis-Godson absorber-weighted mean parameters for temperature and pressure. In spherical geometry the layers may be thought of as concentric shells. In a plane-parallel atmosphere the layers take the form of horizontal slabs (Figure 1).

Paths

Within each layer a series of single gas paths are defined. A single gas path (“path”) is defined along the actual ray trajectory within the layer for each of the different gases comprising the layer. The gas within the layer is assumed homogeneous; a path forms the basic unit for the calculation of optical depth.

Mixed Paths

GENRUN calculates the optical depth for each of the single gas paths within each layer and these are stored individually. The path optical depths are later combined, or mixed, to obtain multi-gas optical depths in a layer, or optical depths over several layers, according to the problem being addressed. A mixed path is therefore defined as a combination of paths either within the same layer or across different layers. By keeping the single gas path optical depths separate, several different mixed path calculations that use the same basic set of path optical depth components can be performed by GENRUN in parallel.

Figure 1 gives an application of these ideas. One mixed path that might be of interest could be formed from the combination of paths 6, 7, 8, 9, and 10 to obtain a mixed path representing the passage of radiation through the CO\(_2\) component of the atmosphere alone. By summing the optical depths of these paths the total CO\(_2\) optical depth is formed. Another calculation might be the combination of paths 4, 9, and 14 to obtain a mixed path representing the passage of radiation through all the gases of layer 4. By summing the optical depths of these paths the total optical depth of layer 4 is obtained.

The main purpose of the layering calculations in GENRUN is to calculate a set of mean gas parameters including temperature, pressure and gas amount, for each of the single gas paths defined by the user input. The line-by-line calculations then proceed for each of the paths.
Figure 1: Decomposition of an atmospheric path of mixed gases into layers and single gas paths.

6.2 Atmospheric Profiles

The atmospheric profile used in the layering calculation can be supplied by the user or taken from one of six zonal- and seasonal-averaged AFGL model profiles [Anderson et al., 1986]. The model profiles are listed in the file glatm.dat. The program also allows a user’s profile, if optionally specified, to be merged with the model profile when necessary data is missing from the former. The program requires vertical atmospheric profiles for pressure [mb], temperature [K], air density [molecules.cm\(^{-3}\)], and gas mixing ratios [ppmv] for each of the gases specified in the input file. The user file is first searched for the mixing ratio profile of a required gas and if it is not present the specified model profile is used. There is also an option to continue the user profile to higher altitudes using the model profile. This is especially useful for continuing experimentally determined mixing ratio data. A vertical profile for the refractive index is calculated from the temperature and pressure profiles. The index of refraction is calculated using the modified Edlén equation of Birch and Downs [1993] as corrected by Birch and Downs [1993]. Also see Edlén [1966].

Altitude [km] is the vertical coordinate used internally by GENRUN. If atmospheric profiles are supplied at pressure levels then a corresponding height is calculated. This is done using the hydrostatic equation taking into account the dependence of air molecular weight on humidity and the variation of gravitational acceleration with altitude and latitude.

6.3 Atmospheric Layering

The atmospheric layer boundaries may be supplied by the user or, alternatively, an optimal set of boundaries are calculated based on a maximum allowed variation of temperature and average Voigt
line half width across a layer. The maximum variations of temperature across the lowest and highest layers are supplied by the user. The allowed temperature variation at middle altitudes is determined by exponentially interpolating between these two values. The choice of temperature variation will depend on the viewing geometry and the required accuracy. It allows a finer layer structure to be calculated at lower altitudes and in the region of a temperature inversion. As a guide, the variation in the lowest layer should be a few degrees, less than 5 $K$, and for most applications, it can be around 20 $K$ for the top layer. The temperature condition determines the accuracy of the GENRUN radiance calculation. This is dependent on the evaluation of the Planck function at the mean layer temperature which should be representative of the temperature within the layer. The fractional variation of Voigt half width across a layer is also set by the user and should have a value between 1 and 2. This condition ensures the accuracy of the transmittance calculation. For some applications it may be necessary to perform sensitivity calculations to ensure that the optimum number of layers is being used for the desired accuracy and speed of computation.

Since the transmittance weighting functions for limb viewing geometries peak near the tangent point, it is important that a fine layer structure be used in this region. A vertical layer thickness of 1 $km$ or less is suggested for the lowest layer.

Once the layer structure is determined, a path is defined for each of the required gases within the layer. The parameters required to define the ray trajectory over the path are the layer boundary altitudes and the local zenith angle at the lower layer boundary, see Figure 2. The initial ray zenith angle at the lower boundary of the atmosphere is supplied by the user. The local zenith angle $\theta$ at the lower boundary of each layer is then calculated according to Snell’s law

$$c = n(r) r \sin \theta,$$

where $c$ is a constant along the ray path and $n(r)$ is the refractive index of air at a radius $r$ from the Earth’s center.
When the ray paths have been fully defined, the Curtis-Godson absorber weighted mean values are calculated for each path \( j \). The integrated absorber amount \( u_j \) for the ray path \( s \) between the vertical layer boundary heights \( z_l \) and \( z_{l+} \) is

\[
u_j = \int_{z_l}^{z_{l+}} \left( \rho_a(z_j) \frac{ds}{dz} \right) dz \tag{8}
\]

where \( \rho_a(z_j) \) is the local number density of gas \( j \). The mean values for the path pressure \( p_j \) and temperature \( T_j \) are

\[
p_j = \frac{1}{u_j} \int_{z_l}^{z_{l+}} p(z) \left( \rho_a(z_j) \frac{ds}{dz} \right) dz \tag{9}
\]

\[
T_j = \frac{1}{u_j} \int_{z_l}^{z_{l+}} T(z) \left( \rho_a(z_j) \frac{ds}{dz} \right) dz \tag{10}
\]

In this way, slightly different values for the layer mean temperature and pressure are obtained for each path gas. The layer is subdivided into several thinner layers in order to perform the in-layer ray tracing and integration. The algorithm used is similar to that used in the LOWTRAN7 code. [Kneizys

Figure 2: Geometry of a limb path through a refractive atmosphere.
et al., 1988]. The temperature and gas mixing ratio are assumed to vary linearly between the layer boundaries, whilst the pressure and density are assumed to vary exponentially.

The layering calculation is set up to perform ray tracing in the Earth’s atmosphere. The calculation of the hydrostatic equation and the refractive index are specific to the Earth. If GENRUN is to be used for layering the atmosphere of a different planet then several modifications will be necessary. The calculation of the Earth’s radius and refractive index in subroutine refrac.f90 will need to be changed, as will the calculation of the gravitational constant in subroutine pressure_height.f90. The lines of code requiring change are indicated by comments in the routines. The atmospheric profiles will have to be supplied in full.

Figure 2 defines the geometry of the raytracing and layering calculation. For a nadir or zenith viewing problem the local zenith angle \( \theta \) at any layer will be zero. For a limb viewing calculation \( \theta=90^\circ \) at the tangent point and decreases with altitude. For a spherically symmetric atmosphere the transmittances in layers either side the tangent point are identical and path parameters are only required from the tangent point to space. The total transmittance from space to the tangent point and back to space again can be formed as a mixed path calculation by doubling the calculated path optical depths from the tangent point to space.

The angle parameters defining the refracted ray path are shown in Figure 2. Each path \( j \) is defined by the zenith angle at the lower layer boundary \( \theta_j \), the path Earth-centered angle \( \beta_j \), the path bending angle \( \Psi_j \), the zenith angle at the upper layer boundary \( \phi_j \), and the path length within the layer \( PL_j \).

For each of the gases for which refractive ray paths are calculated through the atmosphere, the total column amount, total ray path length \( PL_{j, tot} \), total Earth-centered angle \( \beta_{tot} \), and total ray path bending angle \( \Psi_{tot} \) are also given. Derived quantities are written to genln3 ascii_summary.out. They are potentially useful for applications where a detailed path description is needed as input to another calculation. The following four lines illustrate the ray information extracted from genln3_ascii_summary.out for a single path. A detailed description of this record format is given in Section 7.10.

\[
! PATH 75 * O3* HEIGHTS: 5.127 - 5.874 km, 5.500E+02 - 5.000E+02 mb.
! RAY LENGTH = 0.7465 km, THETA = 0.0000E+00.
1, 3, 0, 6.8438334757E-11, 266.96140, 269.44821, 264.44645, 5.1788162117E-01, 5.4280779669E-01,
4.9346163336E-01, 2.0067980604E-08, 'VOIGT ' , 'nocon '
\]

7 The Line-by-Line Calculation: Program GENRUN

7.1 Overview

GENRUN performs the line-by-line calculations. Inputs to the program include the line file produced by HITRUN, the relevant geometry, and a set of homogeneous gas paths each defined by gas amount, temperature and pressure. For atmospheric radiative transfer problems the path data is calculated within GENRUN prior to the radiative transfer modeling. For the simulation of a laboratory experiment the path data might be determined by conditions within a gas cell. The input file also specifies how the optical depths of various paths, once calculated, are to be combined to form mixed paths for transmittance and radiance calculations. The basic stages of the line-by-line calculation are described below.

7.2 Spectral Modeling

The monochromatic absorption coefficient \( k(\nu) \) \([1/(\text{molecules.cm}^{-2})]\) at wave number \( \nu \) \([\text{cm}^{-1}]\) is calculated for each spectral line \( i \) using the line parameters obtained from the HITRUN spectral line file. In the atmosphere, a spectral line is collision and Doppler broadened about the transition wavenumber \( \nu_i \), the spread represented by the normalized line shape function \( g(\nu, \nu_i) \) \([\text{cm}^{-1}]\) such
that
\[ k(\nu) = S_i g(\nu, \nu_i), \]  

(11)
Here \( S_i \) \([\text{cm}^{-1}/(\text{molecules.cm}^{-2})]\) is the line strength adjusted for the local gas temperature. The line strengths and widths are read from the line data files at a standard temperature \( T_{\text{ref}} \) of 296K and pressure \( P_{\text{ref}} \) of 1 atm, and must be adjusted to the path pressure \( p \) and temperature \( T \). The following expression is used to calculate the line strength \( S(T)_i \) from the strength \( S(T_{\text{ref}})_i \), read from the line data file:
\[
\frac{S(T)_i}{S(T_{\text{ref}})_i} = \left( \frac{Q(T_{\text{ref}})}{Q(T)} \right) \left( \frac{\exp(-\frac{hcE_i}{kT})}{\exp(-\frac{hcE_i}{kT_{\text{ref}}})} \right) \left( \frac{1 - \exp(-\frac{hc\nu_i}{kT})}{1 - \exp(-\frac{hc\nu_i}{kT_{\text{ref}}})} \right)
\]  

(12)
Here \( Q(T) \) is the total internal partition function, \( E_i \) in \( \text{cm}^{-1} \) is the energy of the lower state of the transition, \( c \) is the speed of light, \( h \) the Planck constant, and \( k \) the Boltzmann constant. The ratio \( Q(T_{\text{ref}})/Q(T) \) of total internal partition functions is calculated using the parameterization of Gamache et al. [1990]. This is an improvement over the usual classical approximation for the independent temperature variation of the rotational and vibrational components of the partition function. The second factor on the right in Equation (12) accounts for the ratio of Boltzmann populations, and the third for the effect of stimulated emission. The lines strengths in the HITRAN line database are weighted for the natural abundance of the particular isotope in the terrestrial atmosphere. These line parameters may be used in calculations where different isotope abundances apply: in this case the line strength for a given isotope should be divided by the terrestrial fractional abundance and scaled according to the new fractional abundance.

The collision broadened line half width \( \alpha_L(p, T)_i \) in \( \text{cm}^{-1} \) for line \( i \) at pressure \( p \), partial pressure \( p_s \), and temperature \( T \) is calculated as
\[
\alpha_L(p, T)_i = \left( \frac{T_{\text{ref}}}{T} \right)^m \left( \alpha_{La}(p_{\text{ref}}, T_{\text{ref}})_i \left( \frac{p - p_s}{p_{\text{ref}}} \right) + \alpha_{Ls}(p_{\text{ref}}, T_{\text{ref}})_i \frac{p_s}{p_{\text{ref}}} \right),
\]  

(13)
where \( m \) is the positive coefficient of temperature dependence of the air-broadened half width. (In the absence of other data, this coefficient is assumed the same for self-broadening), \( \alpha_{La} \) is the air-broadened half width, and \( \alpha_{Ls} \) the self-broadened half width. For cases where the the self-broadened half width data is absent, GENRUN sets it equal to the air-broadened half width, with the exception of \( \text{H}_2\text{O} \) where \( \alpha_{Ls} = 5 \times \alpha_{La} \) [Burch, 1982]. The user can modify this treatment by examining the code in subroutine \textit{path\_adjust.f90}, where both Eqn 12 and Eqn 13 are calculated.

### 7.3 Line Shape Modeling

Considerable attention has been given to line shape modeling in GENLN3. In the lower atmosphere, pressure broadening of spectral lines is the dominant broadening process. This arises as a result of collisions between molecules producing a deformation of the molecular energy levels. It is most simply represented by the Lorentz line shape [Goody and Yung, 1989]
\[
g_L(\nu, \nu_i) = \frac{1}{\pi} \frac{\alpha_L}{\nu_i^2 + (\nu - \nu_i)^2},
\]  

(14)
The function \( g_L \) \([1/\text{cm}^{-1}]\) agrees well with infrared measurements within a few wavenumbers of the centers of absorbing lines. Other theoretical line shape formulations have also been developed for the treatment of collision broadened lines. Each is derived with a different set of assumptions to describe the mechanism of the collisional process. GENLN3 has provision for calculating the Van Vleck and Huber line shape [Van Vleck and Huber, 1977] extended by Clough et al. [1980]. This is applicable to absorption over the infrared and microwave regions
\[
g_{VVH}(\nu, \nu_i) = \frac{\nu}{\nu_i} \frac{\tanh(hc\nu/2kT)}{\tanh(hc\nu_i/2kT)} \left[ g_L(\nu, \nu_i) + g_L(-\nu, \nu_i) \right].
\]  

(15)
At high altitudes where the pressure is low, Doppler broadening of the spectral lines must be taken into account. This is a result of the velocity distribution of absorbing molecules relative to an observer. The normalized line shape is given by

\[ g_D(\nu, \nu_i) = \frac{1}{\alpha_D \sqrt{\pi}} \exp \left( -\ln 2 \left( \frac{(\nu - \nu_i)^2}{\alpha_D^2} \right) \right) \]  

(16)

where \( \alpha_D \) in cm\(^{-1} \) is the Doppler half width,

\[ \alpha_D = \nu_i \sqrt{\frac{2 \ln 2}{kT}} \frac{mc}{2} \]

(17)

The height at which Lorentz and Doppler broadening become comparable is dependent on the molecular mass \( m \) of the radiating molecule and the wavenumber \( \nu_i \) of the transition. Because this height may be as low as the upper troposphere and since an atmospheric transmittance problem may extend from low to high altitude, it is in general important to consider the combined effect of Lorentz and Doppler broadening. For the 4.3 \( \mu \)m band of \( \text{CO}_2 \) the two broadening mechanisms become comparable at an altitude of about 27 km.

The Voigt profile [Armstrong, 1967] is appropriate to most cases of atmospheric transmittance. It may be regarded as a convolution of the Lorentz and Doppler line shapes and approximates to each in the appropriate limit. The normalized line shape is given by

\[ g_V(\nu, \nu_i) = g_0 K(x_i, y_i), \]

(18)

where

\[ g_0 = \frac{1}{\alpha_D \sqrt{\pi}} \frac{\ln 2}{\sqrt{\pi}} \]

(19)

\[ K(x_i, y_i) = \frac{y_i}{\pi} \int_{-\infty}^{\infty} \frac{\exp (-t^2)}{y_i^2 + (x_i - t)^2} dt \]

(20)

\[ x_i = \frac{\nu - \nu_i}{\alpha_D \sqrt{\ln 2}} \]

(21)

\[ y_i = \frac{\alpha_L}{\alpha_D \sqrt{\ln 2}} \]

(22)

\( K(x, y) \) is known as the Voigt function and is the real part of the complex probability function

\[ w(z_i) = \exp^{-z_i^2} \left( 1 + \frac{2}{\sqrt{\pi}} \int_{0}^{z_i} \exp^{t^2} dt \right). \]

(23)

where \( z_i = x_i + iy_i \). Unfortunately, the Voigt function has no simple analytical solution and must be evaluated numerically. The usual approach is to divide the \( x, y \) plane into several regions and use appropriate functional expansions of the integral in each so as to optimize the combination of accuracy and speed of computation.

Comparisons of line-by-line calculations with measurements taken by high spectral resolution instruments have shown the importance of the finer details of line shape. For some gases the simple Voigt line shape is inadequate. Effects such as line coupling (“line mixing”), non-Lorentzian line wing effects, and continuum absorption must be considered. We discuss the first two below, and the third in the following section.

1) Line coupling occurs (by definition) when collisions between a radiating molecule and broadening gas molecules cause the transfer of population between rotational-vibrational molecular states and a redistribution of spectral intensity within a band. At atmospheric pressures this can easily occur in a Q-branch where the spacing between adjacent rotational levels is less than several \( kT \), the most
apparent effect being a reduction in the absorption coefficient in the wings of the branch. The effect
is also observed in atmospheric P- and R-branches. This may be very important for the strong CO₂
Q-branches used by satellite instruments for atmospheric temperature sounding [Edwards and Strow,
1991].

GENLN3 has an option for including the effect of line coupling in the line-by-line calculation. The
coupling calculation requires a coupling parameter which is essentially an extra line parameter
not included on the HITRAN data base. Rather than modify the HITRAN line data format to
include this parameter, the required coefficients for several CO₂ Q-branches are stored in subroutine
cupdat_mod.f90. These coefficients are calculated from, and are specific to, a given set of lines since they
depend on the line strengths and widths. The file containing the lines for which coupling coefficients
have been calculated, co2_mix.dat, is supplied with the code. These lines contain a flag in the HITRAN
REF field to send the code to look for line coupling data when they are read during a GENLN3
calculation. If the line coupling calculation is going to be used then co2_mix.dat should form the
highest status input data base to program HITRUN.

For line-coupling in GENLN3, the theory of Rosenkranz [1975] gives the normalized line shape
function

\[ g(\nu, \nu_i) = \frac{1}{\pi} \frac{\alpha L_i + (\nu - \nu_i)pY_i}{(\nu - \nu_i)^2} \]  

(24)

where \( Y_i \) is the first-order coupling coefficient

\[ Y_i = 2 \sum_{k \neq i} \frac{d_k}{d_i} \frac{W_{ki}}{\nu_i - \nu_k}. \]  

(25)

Here \( d_k \) and \( d_i \) are dipole matrix elements for lines \( k \) and \( i \) respectively and \( W_{ki} \) is the relaxation
matrix element for coupling between line \( i \) and line \( k \). The \( W_{ki} \) elements are obtained using a
temperature dependent energy-gap scaling law [Strow and Gentry, 1986]. For atmospheric radiative
transfer applications this line shape must be convolved with the Doppler line profile. This gives

\[ g(\nu, \nu_i) = g_0(\mathcal{R}[w(z_i)] + Y_i\mathcal{I}[w(z_i)]). \]  

(26)

This is calculated in subroutine voight_co2.f90. The first term of this expression is the usual Voigt
line shape; the second accounts for line coupling. The complex probability function and therefore the
Voigt function are obtained using the algorithm of [Humlicek, 1982].

The \( Y \)-coefficient is parameterized as a function of temperature \( T \) and pressures \( p \) and \( p_s \) in
subroutine path_adjust.f90:

\[ Y_i(T, p, p_s) = (p - p_s) \left[A_i + B_i \zeta + C_i \zeta^2 + D_i \zeta^3\right] \]
\[ + \quad p_s \left[A_i + B_i \zeta + C_i \zeta^2 + D_i \zeta^3\right] \times \left(\frac{200}{T}\right)^{0.75} \]

(27)

where \( \zeta = T - 200 \). Here the parameters with subscript “a” account for air-broadening, those with
subscript “s” for self-broadening. Parameters \( A, B, C, \) and \( D \) are stored in cupdat_mod.f90 for the
CO₂ Q-branches at 617, 667, 720, 740, and 791 cm⁻¹. The \( Y \)-coefficient is calculated at the same time
that line strength and half width are adjusted for the temperature and pressure of the atmospheric
path under consideration. \( Y \) is then carried in the code as an extra line parameter until the line profile
is calculated according to Equation [26].

2) The sub-Lorentzian nature of the far wings of CO₂ lines is well known (Cousin et al. [1985] and
references therein). Usually, the line shape function \( g(\nu, \nu_i) \) based on the impact theory is multiplied
by a corrective factor \( \chi \) to give an empirical line shape

\[ g(\nu, \nu_i)^{\text{empirical}} = g(\nu, \nu_i)\chi(\nu, \nu_i). \]  

(28)
The $\chi$-factor is a correction to account for the finite duration of collision between the broadening gas and the radiating molecule. This is assumed instantaneous in the impact approximation which forms the basis of most collision broadened line shape theories. It also includes the effect of line coupling far from band center since the $\chi$-factor essentially represents the difference between measurement and Lorentzian line wing theory. The factor usually takes the form of an exponential, with adjustable parameters, and decays from unity at line center. These parameters have traditionally been chosen by fitting the calculated absorption to the measured absorption in the region above the $CO_2 \nu_3$ band head at 4.3$\mu$m. The $\chi$-factors calculated in this region are often used in $CO_2$ line shapes at other vibrational bands. The user should be aware that the component of the factor due to line coupling will then be in error as it is dependent on the symmetry of the vibrational levels connected by the transition through the number of available final rotational states. This is not usually a problem as the exponential part of the $\chi$-factor due to duration of collision effects quickly dominates the contribution due to coupling. Birnbaum [1979] suggested a $\chi$-factor comprising the product of a decaying exponential to account for the finite duration of collisions alone and a constant term for line coupling. The exponential term should be band independent while the constant coupling term will not. This is discussed further in Edwards and Strow [1991].

GENLN3 includes a $CO_2$ line shape option that includes the effect of line coupling and sub-Lorentzian line wings. If data is available, line coupling is included explicitly according to Equation [26] out to an arbitrary 10 cm$^{-1}$ from line center. The line wings at greater distances from line center are modified by the temperature dependent $\chi$-factor of Cousin et al. [1985]. If line coupling data is not available then this sub-Lorentzian line shape is used everywhere.

### 7.4 Continuum Absorption

Along with line-by-line absorption, the continuum absorption of certain molecules, in particular water vapor, must also be considered. Continuum data are available for $H_2O$, $CO_2$, and the $N_2$ and $O_2$ pressure broadened bands. The continuum calculations are called through subroutine `contum.f90`.

#### 7.4.1 $H_2O$

Accurate modeling of $H_2O$ is especially important in remote sensing applications which utilize the infrared atmospheric windows near 4 $\mu$m and 8-12 $\mu$m. The $H_2O$ continuum is responsible for most of the absorption in these regions and the large seasonal and zonal variations in $H_2O$ mixing ratio in the troposphere can lead to a wide range of calculated attenuations. Water vapor continuum absorption has sometimes been called “anomalous” because it is not accounted for by line shapes based on simple collision broadening theory and having Lorentzian wings. The continuum may be considered as making up the difference between the observed absorption and that resulting from a sum over all $H_2O$ spectral lines in the atmospheric window regions that are located near strong water bands. Thus its definition will depend on the reference line shape chosen, and this, along with the spectral region of interest, will determine if the continuum represents a “surplus” or “deficit” of absorption. The continuum formulation is therefore inextricably linked to the line shape description and the lack of formal agreement on definition has led to confusion and hindered comparison of different models [Clough et al., 1989b].

Despite much effort there is still no comprehensive theory to account for the $H_2O$ continuum. It is essentially broadband, decreases rapidly with temperature, and in the 8-12 $\mu$m window is much stronger for pure water vapor where self-broadening effects are important than for air-broadened lines. Further technical discussion is given in [Edwards, 1992].

The need for a continuum absorption parameterization that can be used in radiative transfer models has led to the adoption of a semi-empirical approach. The model of Clough et al. [1980, 1989b] has been used in FASCODE [Clough et al., 1989a], LOWTRAN [Kneizys et al., 1988], and is used in GENLN3. It describes the far line wings using the Van Vleck and Huber impact approximation line
shape modified by an empirically determined factor to fit the calculated absorption to the experimental data of Burch and Alt [1984].

The continuum absorption coefficient $k_c(\nu)$ due to all lines $i$ is defined by

$$k_c(\nu) = \nu \tanh \left( \frac{hc\nu}{2kT} \right) \sum_i S_i \nu_i \tanh(\frac{hc\nu_i}{2kT}) (g_c(\nu, \nu_i)\chi(\nu, \nu_i) + g_c(-\nu, \nu_i)\chi(-\nu, \nu_i))$$

(29)

with $\chi(\nu, \nu_i)$ defined in Equation [28] and

$$g_c(\pm \nu, \nu_i) = \frac{1}{\pi} \frac{\alpha L}{\alpha^2 L + (\nu \pm \nu_i)^2} \text{ for } |\nu \pm \nu_i| \geq 25 \text{ cm}^{-1}$$

(30)

$$g_c(\pm \nu, \nu_i) = \frac{1}{\pi} \frac{\alpha L}{\alpha^2 L + 25^2} \text{ for } |\nu \pm \nu_i| \leq 25 \text{ cm}^{-1}$$

(31)

This description includes a constant continuum component over the line center region to avoid a discontinuity at 25 cm$^{-1}$ from line center. This component must be remembered when performing the line-by-line calculation out to 25 cm$^{-1}$ from line center so that it is not counted twice.

Equation [29] may be written

$$k_c(\nu) = \nu \tanh \left( \frac{hc\nu}{2kT} \right) C(\nu)$$

(32)

where $C(\nu)$ is the wavenumber dependent continuum parameter. For water vapor in the infrared, $\chi = 1$ within about 5 cm$^{-1}$ of the line center. At greater distances up to about 500 cm$^{-1}$ the line shape becomes super-Lorentzian. The $\chi$ factor depends on $|\nu - \nu_i|$ and approaches values as large as 10 for the self-broadened case. At greater distances still the line becomes sub-Lorentzian. Similar behavior is found in the air-broadened case though to a lesser extent, with $\chi > 1$ up to about 100 cm$^{-1}$ from line center.

Applying this definition of the continuum, the total continuum contribution to the absorption coefficient $k_c(\nu)$ can be written

$$k_c(\nu) = \nu \tanh \left( \frac{hc\nu}{2kT} \right) \left( \frac{T_{ref}}{T} \right) \left( \frac{p_s}{p_{ref}} \left( C_s^0(\nu, T) + \frac{(p - p_0)}{p_{ref}} C_f^0(\nu, T) \right) \right).$$

(33)

Here $C_s^0$ is the continuum absorption parameter for the self component and $C_f^0$ the parameter for the foreign component, with units $1/(cm^{-1}molecules.cm^{-2})$. $C_s^0$ and $C_f^0$ are defined at the reference pressure $p_{ref}$. The temperature and pressure factors in Equation [33] take into account the density dependence of the self and foreign broadened line half widths. Values of $C_s^0$ are stored in the code at temperatures of 260 K and 296 K. The strong negative temperature dependence is obtained by exponentially extrapolating between these values at the required wavenumber. Due to a lack of measurements at lower temperatures, the 260 K data is a downward extrapolation of Burch’s measurements at 296 K and 338 K and as such is a potential source of error. The temperature dependence of $C_s^0$ has not been determined and room temperature values are used.

The line-by-line part of the GENLN3 calculation takes into account line wings up to 25 cm$^{-1}$ from line center. The pre-computed continua described here account for the absorption contribution of the line wings at greater separations.

**7.4.2 CO$_2$, O$_2$, N$_2$**

A CO$_2$ continuum is calculated using the GENLN3 CO$_2$ line shape. This is stored in the code at temperatures of 230 K, 250 K and 296 K and the absorption at a particular path temperature is obtained by interpolation between these values at the required wavenumber.

The pressure broadened bands of N$_2$ at 2350 cm$^{-1}$ [Clough et al., 1981] and O$_2$ at 1550 cm$^{-1}$ [Timofeyev and Tonkov, 1978; Rinsland et al., 1989] are included as broad-band continuum contributions to the absorption. The same facility may be used to include other grey absorptions such as aerosols.
7.5 Molecular Cross-Section Data

High resolution cross-section data are used to calculate absorption by molecules for which line data is not available. HITRAN currently provides cross-sections for several dozen molecules. These are readily accessed and used by GENLN3. Examples are given in Section 8.

7.6 Aerosol Model

A sulfate ($H_2SO_4$) aerosol calculation is implemented in subroutine aeroab.f90. Aerosol extinction $[km^{-1}]$ is calculated using a fixed extinction profile at reference wavenumber $\nu_{ref}$. This profile is tabulated under GASID 91 in file glatm.dat. The profile describes aerosol loading prior to the Mt. Pinatubo eruption and provides a low-aerosol climatology. An alternative high-aerosol climatology (post-Pinatubo) is also in the file and may be used instead by manually commenting-out/uncommenting the low/high-aerosol case. The GENLN3 file aero.dat contains pre-computed tables of sulfate aerosol extinction as functions of wavenumber and temperature $T$ for a reference aerosol amount $A_{ref}$ derived from Mie calculations. In aeroab.f90 the local $T$ and $\tau_{H_2O}$ at each altitude are used to interpolate within these tables, yielding extinction spectra for amount $A_{ref}$. The spectra are then rescaled to match the given aerosol extinction profile at $\nu_{ref}$. This yields aerosol extinction spectra as functions of wavenumber and height which are then folded readily into the rest of the GENLN3 calculation. Sulfate is the only aerosol currently included in GENLN3. An example calculation which includes sulfate aerosol is given in Section 8.

7.7 The Line-By-Line Calculation

The line-by-line calculation involves calculating transmittances over the spectral range of interest in wavenumber space for each gas in several atmospheric layers. The simplest procedure is to choose a wavenumber grid fine enough that the narrowest line is adequately sampled, typically 0.0005 cm$^{-1}$. Then for each line $i$ of path gas $j$ taken in turn the monochromatic absorption is calculated at each grid point over the whole wavenumber range. The absorption coefficient at a wavenumber $\nu$ can be written as the sum over the absorption contributions from all lines $i$ in the spectral range,

$$k(\nu)_j = \sum_i S_{ij} g(\nu, \nu_i)_j$$

(34)

Here $S_{ij}$ is the strength of line $i$ adjusted to the conditions of path $j$ and $g(\nu, \nu_i)_j$ is the line shape function. The total transmittance of a mixed path comprising $J$ single gas paths over several layers of the atmosphere is then

$$\tau(\nu) = \exp \left( - \sum_{j=1}^{J} k(\nu)_j u_j \right) = \prod_{j=1}^{J} \exp (-k(\nu)_j u_j)$$

(35)

where the path gas amount $u_j$ in $molecules.cm^{-2}$ is defined in Equation [8]. Equation [35] is the approximation used to calculate the integral of Equation [3]. As discussed in Section 5.2, HITRUN scales the line strength by the Avogadro number $6.022 \times 10^{26} [molecules/kmole]$, therefore gas amounts in the GENRUN input file are stated in $kmole.cm^{-2}$ to compensate.

To calculate the absorption coefficient for every line at every wavenumber grid point is prohibitive for most applications and represents an excessive amount of computer time and storage. Most algorithms that speed up the computation work on the basis that a wider wavenumber grid may reasonably be used in the wings of lines whilst a fine grid is required over the line center where the line profile is changing rapidly. The calculation also only needs to be performed for lines of significant strength.

In GENLN3 the spectral calculation is fully specified by the user input (Figure 3). The wavenumber range is first divided into a number of “wide mesh” intervals which may be of constant or variable
spacing. The line-by-line multi-path calculation proceeds in two stages. For each gas path a “wide-pass” is first made over the total spectral range. For each wide mesh in turn, the absorption due to the wings of lines whose centers fall into the range $f_{\text{exc}}$ to $f_{\text{wind}}$ from the wide mesh boundaries are computed at the lower boundary, center, and upper boundary of the interval. The absorption contribution of the wings of lines whose centers are further than $f_{\text{wind}}$ from the wide mesh boundary are included by means of a precomputed temperature dependent continuum described in the next section. The contribution of far line wings and of lines lying outside of the wavenumber range of interest is important, especially near strong absorption bands [Fischer et al., 1991]. When the absorption contributions from all far-off line wings have been considered, a quadratic interpolation between the three values at the wide mesh wavenumber points gives the total line wing absorption at intermediate points.

![Diagram of GENLN3 spectral calculation scheme](image)

**Figure 3:** The GENLN3 spectral calculation scheme.

A “fine-pass” is then made over a fine wavenumber grid obtained by sub-dividing the wide mesh interval into many smaller intervals. This absorption calculation is performed for close lines where the line shape may be changing very rapidly. All lines whose centers lie within $f_{\text{exc}}$ of the wide mesh boundaries are included. The number of fine grid points within each wide mesh interval defines the resolution of the calculation and is determined by the width of the narrowest line encountered.

25
The interpolated wide-pass absorptions at the fine grid wavenumber points are then added to the fine-pass absorptions at these same points. This gives the line absorption totals within each wide mesh interval.

GENLN3 includes a line selection so that the line-by-line calculation is not performed for extremely weak lines. The minimum line strength is determined as follows. An Elsasser distribution of lines [Goody and Yung, 1989] of half width 0.1 cm\(^{-1}\), peak separation 0.01 cm\(^{-1}\) and constant strength S, is assumed to represent the extreme case of a tight absorption band of low optical depth. If for path \(j\) the transmittance of such a line distribution is greater than 0.99999, then the lines are not considered significant. This condition implies a minimum value of \(S_ju_j\) for the line to be used. The wide-pass stage of the calculation rejects lines for which \(S_ju_j < 10^{-7}\) and the fine-pass stage rejects lines for which \(S_ju_j < 10^{-8}\). These values are set in subroutines \textit{widepass.f90} and \textit{finepass.f90} with the variable \(stmin\). To perform the calculation using all lines, \(stmin\) should be set to zero. The user should be aware that this condition for line rejection is only relevant for lower and middle terrestrial atmosphere studies and should be changed if GENLN3 is used for other applications.

Transmittances are required over the spectral range of interest for each single gas path in the several tens of atmospheric layers. To store the absorption coefficients for the whole spectrum for all paths would result in prohibitively large array sizes. GENLN3 performs a “vertical” calculation in which the absorption coefficients are calculated for all paths in all layers but are only stored for each wide mesh interval before being written to output. Thus at any one time the monochromatic optical depths of all gas paths in all layers are known for one wide mesh interval.

### 7.8 Transmittance Calculations

Having calculated the various components contributing to absorption at the fine grid wavenumber points for some path \(j\), the total monochromatic absorption coefficient may be formed,

\[
k(\nu)_j = k(\nu)_j^{\text{line-wings}} + k(\nu)_j^{\text{near-lines}} + k(\nu)_j^{\text{broadband}}
\]  
\[(36)\]

The broadband absorption includes the continuum and molecular cross-section contributions. The monochromatic optical depth of the path is given by the product of the absorption coefficient and the total path absorber amount \(k(\nu)_j u_j\). At this stage the optical depths of the various single gas paths may be combined to obtain multi-gas optical depths and optical depths over several layers according to the problem being addressed. This operation is performed in GENLN3 by a device called a \textit{mixing table}, here represented by the matrix \(M\). The elements \(M_{m,j}\) specify the contribution that each path optical depth \(k(\nu)_j u_j\) is to make in forming the mixed path optical depth \(K(\nu)_m\) for some mixed path \(m\). If there are \(N_m\) mixed path absorptions to be formed from the \(N_p\) computed path absorptions the calculation takes the form

\[
\begin{pmatrix}
K(\nu)_1 \\
K(\nu)_2 \\
\vdots \\
K(\nu)_{N_m}
\end{pmatrix} =
\begin{pmatrix}
M_{1,1} & M_{1,2} & \cdots & M_{1,N_p} \\
M_{2,1} & M_{2,2} & \cdots & M_{2,N_p} \\
\vdots & \vdots & \ddots & \vdots \\
M_{N_m,1} & M_{N_m,2} & \cdots & M_{N_m,N_p}
\end{pmatrix}
\begin{pmatrix}
K(\nu)_1 u_1 \\
K(\nu)_2 u_2 \\
\vdots \\
K(\nu)_{N_p} u_{N_p}
\end{pmatrix}
\]  
\[(37)\]

This calculation is performed over each point of the fine wavenumber grid. The transmittance of each mixed path is then calculated according to

\[
\tau(\nu)_m = \exp(-K(\nu)_m)
\]  
\[(38)\]

The mixing table is a versatile device which allows for economy of calculation of many atmospheric mixed paths. For example, slant path calculations through the atmosphere for a series of small angles may be simply performed by multiplying the vertical path absorptions by \(\sec \theta\), where \(\theta\) is the local zenith angle. Such a calculation does not take into account refraction effects but this is not found to be a serious source of error for values of \(\theta\) less than about 60°. It represents a considerable economy
of calculation when several slant path views for the same atmospheric profile are to be computed. The mixing table is also very useful for performing several transmittance calculations in parallel for slightly different atmospheric profiles. If the profiles have paths in common then the optical depths of these need only be computed once and combined with the path absorptions of other gases in the mixed paths as required. An application of this might be in determining the sensitivity of the atmospheric absorption to differing amounts of one particular gas, the mixing ratio profiles of the other gases remaining constant.

An example mixing table is shown in Figure 4 along with an illustration of the mixed paths it calculates. The table uses the set of 15 paths shown in the example of Figure 1 and defined by the mixing table above it. Mixed path 1 shows how the optical depths of several layers may be combined for a single gas. This mixed path may be used to find the transmittance of the atmosphere due to water vapor alone. Mixed paths 2 – 4 are for a calculation to investigate the attenuating effect of mixed gas absorption from different levels in the atmosphere. Mixed paths 5 – 6 represent a slant path calculation for a zenith angle of $\theta = 45^\circ$. Mixed paths 7 – 11 calculate the total optical depth for each layer of the atmosphere. These mixed paths could be used to represent the layer in a GENLN3 radiance calculation in the way described in the next section. The example shown here is for a nadir viewing geometry. For a limb-viewing geometry the mixing table is used to combine path optical depths for different gases within a layer and between layers in the same manner.

GENLN3 has an important and convenient option for satellite applications that by-passes the need to explicitly construct mixing tables in the input file. This is accomplished by assigning the value LIMB, NADIR, FLUX, or CELL to the MODE keyword: these assignments automatically calculate the mixing tables at run time. If the user wishes to explicitly specify paths and mixed paths, setting the MODE to PATH is used together with a mixing table. PATH provides the most flexibility and control over the radiative modeling, as well as backwards compatibility with GENLN2 calculations that required mixing tables. Calculations illustrating the use of LIMB, NADIR, PATH, FLUX, and CELL are found in Section 8.
<table>
<thead>
<tr>
<th>Mixed Path number</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>2</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
<tr>
<td>3</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>4</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>0.0</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>0.0</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>6</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>0.0</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
<td>1.4</td>
</tr>
<tr>
<td>7</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>8</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>9</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>10</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>11</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>1.0</td>
<td>0.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

### Purpose of the Mixed Paths:

1. H₂O only Mixed Path through all layers of the atmosphere
2-4. Mixed Paths from different levels to the top of the atmosphere for all gases
5-6. Slant Mixed Path at θ=45 deg from different levels to top of the atmosphere for all gases
7-11. Single layer Mixed Paths for all gases

---

**Figure 4:** Illustration of mixed paths formed from the paths of Figure 1 and defined by the mixing table above.
7.9 Radiance Calculations

GENLN3 may be run in one of two modes, for transmittance calculations only or for transmittance and radiance. A typical nadir viewing problem in satellite remote sensing might be the calculation of radiance at some altitude \( z_{\text{obs}} \) above the Earth due to the combined effect of a radiating surface at \( z_s \), such as the land, sea or cloud top and the thermal emission of the atmosphere. The observed radiance is given by Equation [6],

\[
I(\nu, z_{\text{obs}}) = I(\nu, z_s) \tau(\nu, z_s, z_{\text{obs}}) + \int_{z_s}^{z_{\text{obs}}} B(\nu, T(z))k(\nu, z)\rho_a(z)\tau(\nu, z, z_{\text{obs}})dz \tag{39}
\]

where \( I(\nu, z_s) \) is the intensity of radiation leaving the surface, \( \rho_a \) is the absorbing gas density, and \( B(\nu, T) \) is the Planck emission function at temperature \( T \). In general \( I(\nu, z_s) \) is given by

\[
I(\nu, z_s) = \epsilon B(\nu, T_s) + (1 - \epsilon) \left( B(\nu, T_b)\tau(\nu, z_b, z_s) + \int_{z_s}^{z_b} B(\nu, T(z))k(\nu, z)\rho_a(z)\tau(\nu, z, z_{\text{obs}})dz \right) \tag{40}
\]

where \( \epsilon \) is the emittance and \( T_s \) the surface temperature. The effective edge of the Earth’s atmosphere is \( z_b \), and \( T_b \) is the temperature at this boundary. The first term on the right-hand side of Equation [40] is the thermal emission of the surface. Assuming specular reflection, the second term is the reflectance multiplied by the total radiation reaching the surface from the atmosphere and boundary. The second term is zero if the surface is a blackbody with \( \epsilon = 1 \). For a limb viewing case looking into cold space, the observed radiance will be due to atmospheric thermal emission alone and will be given by an expression similar to Equation [39] with the first term set to zero and \( z_b \) substituted for \( z_s \).

In the GENLN3 radiance calculation the atmosphere is considered sub-divided into a number of homogeneous layers. The total optical depth of each layer \( l \) is defined in the GENLN3 input from among the computed path optical depths \( k(\nu)_j u_j \) or mixed path optical depths \( K(\nu)_m \). Assuming that the layer is made up of \( J \) single gas paths, the total layer optical depth \( \psi(\nu)_l \) will be given by a mixed path \( m \) for which

\[
\psi(\nu)_l = K(\nu)_m = \sum_{j=1}^{J} k(\nu)_j u_j \tag{41}
\]

and the layer transmittance is

\[
\tau(\nu)_l = \exp(-\psi(\nu)_l) \tag{42}
\]

Each layer also has an associated temperature \( T_l \) which is an absorption weighted mean of the path temperatures that constitute the layer. For a layer in local thermodynamic equilibrium this allows the layer thermal emission \( E(\nu)_l \) to be defined from the integral in Equation [39] and Equation [8] as

\[
E(\nu)_l = B(\nu, T_l) \sum_{j=1}^{J} k(\nu)_j \rho_a \int_{z_{l-}}^{z_{l+}} \tau(\nu, z, z_l)dz = B(\nu, T_l) \left( \frac{\phi(\nu)_l}{\psi(\nu)_l} \right) [1 - \tau(\nu)_l] \tag{43}
\]

where

\[
\phi_l = \sum_{j=1}^{J} k(\nu)_j u_j. \tag{44}
\]

The optical depth ratio \( \phi(\nu)_l/\psi(\nu)_l \) is unity as it stands, but has been retained here to demonstrate how GENLN3 performs an emission calculation. It is often useful to know what component of the
total radiance at some point in the atmosphere is due to the emission from one particular gas species. For example, it is necessary to know how much of the measured instrument signal in a $CO_2$ sounding channel is due to a contaminating $O_3$ signal. Consider a calculation to find the radiance due only to gas $C$ when the atmosphere is composed of gases $A, B, C$ and $D$. Whatever the emission source, it will be attenuated by the layer transmittance $\tau(\nu)_l$ which is defined by the layer optical depth $\psi(\nu)_l$ of all the gases $A, B, C$ and $D$. The optical depth of gas $C$ alone is then used to define the layer emission, i.e. $\phi(\nu)_l = k(\nu)_C u_C$ only. For such a GENLN3 calculation, the user must define in each layer a total optical depth $\psi(\nu)_l$ and the emission source optical depth $\phi(\nu)_l$ by choosing from among the previously calculated path and mixed path optical depths. The radiance calculation then proceeds in two stages. First Equation [40] for the radiation leaving the surface is evaluated if it is defined by the problem. The radiance at the point of observation is then calculated using Equation [39]. In both cases the same step-wise algorithm is used to calculate the radiance at the furthest boundary of the $l^{th}$ layer as

$$I(\nu)_l = I(\nu)_{l-1} \tau(\nu)_l + E(\nu)_l$$  \hspace{1cm} (45)

GENLN3 allows several radiance calculations to be performed at once. Each calculation is specified by the layer optical depths which define the radiating atmosphere, and the boundary temperatures and emittances where appropriate.

7.10 Description of the GENRUN Input File

GENRUN reads a user-supplied input file formatted as described in Section 4.3.

*TITLES

This block is mandatory.

$TITLE (string)$ is the title of the GENLN3 run. This is used as a header for the output files and should be descriptive.

*GEOMET

This block is mandatory.

The GEOMET block contains the important keyword “MODE”. It allows simplified calculations to be set up that avoid the need to explicitly construct mixing tables (by specifying NADIR, LIMB, FLUX, or CELL). It also permits GENLN3 to be run much like GENLN2 (by using PATH).

The MODE keyword takes one of the following values:

NADIR - Calculation using internally-generated mixing tables in nadir geometry.

LIMB - Calculation using internally-generated mixing tables in limb geometry.

PATH - Reads input files containing information similar to GENLN2 format. In particular, user-supplied mixing tables are required. This is the closest GENLN3 offers to GENLN2 input formatting.

CELL - Transmittance calculations requiring user-specified path data, as might be obtained with laboratory measurements. The file format is described below under CELL_FILE_NAME.

FLUX - Flux calculations

$CELL_FILE_NAME$ (string) - Name of the file containing the path data used in a CELL calculation. Mandatory if MODE equals CELL. File ct.path in Section 8.5.3 is an example of the required file format. Each path in the file is a single record. The file format and record format are described below. This is also the format of the gas path output mentioned Section 6.3, derived from the ray tracing, that is written to genln3_ascii_summary.out.

The first record of the path data file contains two fields (e.g. ct.path). The first field ("NPATH") is an integer defining the number of paths to be read.

The following section is then repeated NPATH times.

One or more comment records beginning with "!".

A record consisting of two lines giving the path data, having the the following fourteen fields. The first twelve fields are on one line, the remaining two fields occupy a second line.
1) Integer specifying which line data file or cross-section data file is the source for the path gas information.
2) Integer giving the molecular ID of the path gas.
3) Integer specifying the HITRAN isotope abundance ID defined as follows: if 0, lines of all isotopes of the gas are considered; if 1, lines of the most abundant isotope are taken, and so on.
4) The path integrated gas amount \( [\text{kmoles/cm}^2] \).
5) The average path temperature \([\text{K}]\).
6) The lower boundary temperature \([\text{K}]\).
7) The upper boundary temperature \([\text{K}]\).
8) The average path pressure \([\text{atm}]\).
9) The path pressure at the lower boundary \([\text{atm}]\).
10) The path pressure at the upper boundary \([\text{atm}]\).
11) The average partial pressure of the path gas \([\text{atm}]\).
12) The path velocity relative to the line of sight \([\text{m/s}]\). Currently not implemented; set it to zero.
13) A string specifying the line shape (e.g. ‘VOIGT’).
14) A string specifying if a continuum calculation is performed (‘CON’ or ‘NOCON’).

\$ \text{ATM\_BOUND} \text{ (string)} \) - Specifies the units (height ‘H’ or pressure ‘P’) describing the atmosphere.
\$ \text{ATM\_LOWER\_BOUND} \text{ (real)} \) - Location of the atmosphere lower boundary (height or pressure).
\$ \text{ATM\_UPPER\_BOUND} \text{ (real)} \) - Location of the atmosphere upper boundary (height or pressure).
If height coordinates are used, ATM\_LOWER\_BOUND must be less than ATM\_UPPER\_BOUND.
If pressure coordinates are used, ATM\_LOWER\_BOUND must be greater than ATM\_UPPER\_BOUND.
\$ \text{VIEW\_ZENITH} \text{ (real)} \) - Value of the initial ray zenith angle at the lower atmospheric boundary.
\$ \text{VIEW\_AZIMUTH} \text{ (real)} \) - Value of the initial ray azimuth angle at the lower atmospheric boundary.
\$ \text{TEMP\_UPPER\_BOUND} \text{ (real)} \) - Temperature at atmosphere upper boundary.
\$ \text{TEMP\_SURFACE} \text{ (real)} \) - Surface temperature.
\$ \text{EMISSIVITY\_SURFACE} \text{ (real)} \) - Surface emissivity.
\$ \text{SUN\_ZENITH} \text{ (real)} \) - Solar zenith angle.

\*\text{PTHFIL} \)
This block is mandatory whenever MODE is not equal to CELL. For a CELL calculation this block is not included.

\$ \text{USER\_PROFILE} \)
This keyword must be present if and only if \$ \text{MODEL\_PROFILE} \) is not specified, in which case it is mandatory. If \text{USER\_PROFILE} \) is supplied then PROFILE\_FILE\_NAME \text{(string)}, the file name of the user’s profile data set, is required, and the profile data must be arranged as shown in Figure 5. A description of this file format is given next.
Figure 5: Example of profile data set required with keyword USER_PROFILE.

Header records: The profile file may have title header records beginning with "!". These are printed in the output file so they should be fully descriptive of the profile. The input parameters in the records that follow are read in free format.

First input record:

The first parameter is the character 'H' or 'P'. This specifies whether the profile is supplied on height or pressure levels. The second parameter is the number of profile levels that follow (39 here). The third parameter is the number of gas mixing ratio profiles supplied (4 gas profiles here).

Second input record:
A list of the gas ID’s for which mixing ratio profiles are supplied (4 profiles: gas ID 1 (H₂O), 2 (CO₂), 3 (O₃), 52 (CFC12)).

Third input record:
The first parameter is the Earth latitude where the profile was taken (45° in this case), the second parameter is the height of the first profile level (0.0 km), the third parameter gives the units of the profiles (either ‘ppmv’ or ‘ppv’ is required). If ‘ppv’ is specified the code internally multiplies the given profile values by 10⁶.

Profile records:
There then follows a record for each of the 39 levels. If the profile is defined on height levels (’H’) the first parameter is the height [km]. This parameter is absent if the profile is defined on pressure levels (’P’). Next are the level pressure [mb] and the level temperature [K]. The volume mixing ratio [here ppmv] for each of the specified gases then follow in turn (i.e. ppmv of H₂O followed by ppmv of CO₂ and so on).

If the profiles are supplied only on pressure levels, the corresponding altitudes are calculated in subroutine pressure_height.f90.

$ FLAG_ADD_ON - Specifies if a file is supplied to provide gas profiles that are not present in the user’s profile.

$ ADD_ON_FILENAME (string) - The name of the file containing the model atmospheres being used. These provide mixing ratio profiles that are not present in the user’s profile. The six AFGL model atmospheres [Anderson et al., 1986] are in the file glatm.dat.

$ ADD_ON_PROF_NUMBER (integer) - The number identifying the model atmosphere to be used.

This completes discussion of the $ USER_PROFILE description.

If MODEL_PROFILE is specified (and USER_PROFILE not specified) the following are mandatory:

$ MODPRO_FILE_NAME (string) - The name of the file containing the model atmospheres formatted as described above for the user profile.

$ PROFILE_NUMBER (integer) - The number identifying the model atmosphere to be used.

This completes discussion of the MODEL_PROFILE description.

$ USER_LAYERS
This keyword should be supplied if and only if $ DEFAULT_LAYERS is not supplied, in which case it is mandatory. It allows the user to define the layer boundaries used in the calculation.

$ LAYER_BOUND (string) - Specifies whether the layer boundaries will be given at height 'H' or pressure 'P' levels.

$ LAYER_NUMBER (integer) - The number of layers for calculation.

$ SUB_LAYER_NUMBER (integer) - Determines the number of sub-layers used in performing the Curtis-Godson path integrations. The width of a sub-layer ∆l is given by

\[ \Delta l = \frac{\Delta L}{\text{SUB_LAYER_NUMBER}} \times \cos \theta \] (46)

where ∆L is the total layer width and cos θ is the cosine of the local zenith angle. Setting this keyword to approximately 10 should be adequate.

$ LAYER_TABLE - Flags the start of the user-specified list of layers. The number of values read is LAYER_NUMBER. Each record in the table has the following format;

layer index, height_min, height_max

or

layer index, pressure_max, pressure_min

This completes discussion of the $ USER_LAYERS description.

$ DEFAULT_LAYERS
This keyword is used if and only if USER_LAYERS is not supplied, in which case it is mandatory. It allows the layer boundary heights to be internally calculated by the code.

$ \text{SUB\_LAYER\_NUMBER (integer)}$ - Determines the number of sub-layers used in performing the Curtis-Godson path integrations. (This keyword also appears above with USER_LAYERS).

$ \text{MAX\_VAR\_VOIGT\_HW (real)}$ - The maximum allowed fractional variation factor for an average Voigt half width across a layer. This value should be between 1 and 2.

$ \text{MAX\_TEMP\_DIFF\_BOT (real)}$ - The maximum allowed variation of temperature [K] across the lowest atmospheric layer.

$ \text{MAX\_TEMP\_DIFF\_TOA (real)}$ - The maximum allowed variation of temperature [K] across the highest atmospheric layer. The Voigt half width is calculated for a representative gas of molecular weight 36 and air-broadened half width of $0.1 \text{ cm}^{-1}$ at 1 atm and 296 K. The allowed temperature variation at an intermediate altitude is obtained by exponentially interpolating between MAX_TEMP_DIFF_BOT and MAX_TEMP_DIFF_TOA.

This completes discussion of the $ \text{DEFAULT\_LAYERS description.}$

$ \text{REFRACTION}$ - If this keyword is present then include atmospheric refraction in the calculation.

*DEFGRD
This block is mandatory.

$ \text{MINIMUM\_WAVENUMBER (real)}$ - The minimum wavenumber of any line to be considered in the calculation. This is named “FMIN” in Figure 3.

$ \text{LOWER\_INT\_BOUND (real)}$ - The lower passband wavenumber. This is named “FBDY(NPL)” in Figure 3.

$ \text{UPPER\_INT\_BOUND (real)}$ - The upper passband wavenumber. This is named “FBDY(NPU)” in Figure 3.

$ \text{MAXIMUM\_WAVENUMBER (real)}$ - The maximum wavenumber of any line to be considered in the calculation. This is named “FMAX” in Figure 3.

$ \text{WIDE\_INTERVAL\_SPACING (real)}$ - The constant wide mesh interval spacing. This should have a value of about $1 \text{ cm}^{-1}$ for accurate interpolation of the wing absorption during the fine pass stage. This is named “DELTA” in Figure 3.

$ \text{WN\_RANGE\_FOR\_FINE (real)}$ - The wavenumber range either side of a wide mesh interval for which the fine pass calculation is performed. This is named “FEXC” in Figure 3.

$ \text{WN\_RANGE\_CONSIDER (real)}$ - The wavenumber range either side of a wide mesh interval outside of which lines are not considered. It should be set equal to $25 \text{ cm}^{-1}$ if a continuum absorption calculation is to be performed as discussed in Section 7.4. This is named “FWIND” in Figure 3.

$ \text{DIVISION\_WIDE\_FINE (integer)}$ - Determines the spectral resolution of the calculation. If DIVISION\_WIDE\_FINE is positive, the wide mesh interval is divided into that many fine mesh intervals over which the spectrum is calculated. The line-by-line calculation is then performed on a grid with spacing WIDE\_INTERVAL\_SPACING / DIVISION\_WIDE\_FINE. If DIVISION\_WIDE\_FINE is negative, then the wide mesh interval is divided such that the fine mesh grid spacing is set equal to the minimum path adjusted line width encountered in the current wavenumber range divided by the absolute value of DIVISION\_WIDE\_FINE. This can lead to different fine grid spacings in different wide mesh intervals. In this case, care is required (for example) if the calculated spectra are to be convolved with an instrument function.

$ \text{NUM\_PER\_HALFWIDTH (real)}$ - The number of Voigt width fractions per wide mesh. This is used in the finemesh reduced calculation. It is ignored if assigned the value $-1$.

*GASFIL
This block is mandatory and specifies where the line data files are to be found and which gas lines are to be read from which file. These line data files are the F90 binary unformatted direct access files produced by HITRUN. Any gases described by cross-section data are not included in this block, but instead are listed separately in the *XSCFIL block.

$ \text{NUMBER\_OF\_FILES (integer)}$ - The number of line data files used in the line-by-line calculation.
$GAS\_FILE\_NAME$ - Flags the list of line data files. This keyword is follows by a list containing
$NUMBER\_OF\_FILES$ line data filenames (string).

$NUMBER\_OF\_GASES$ (integer) - Indicates that an integer list follows, specifying how many gases
(listed in the order of the GAS\_TABLE) are read, in turn, from the line file(s) under GAS\_FILE\_NAME.

$GAS\_TABLE$ - Flags the list of gases used in the calculation. This keyword is followed by a
series of records each containing five fields. These are defined as follows:

The first field (integer) is the gas molecular ID.

The second field (integer) is the HITRAN isotope abundance ID defined as follows: if assigned "0"
then lines of all isotopes of the gas are considered; if assigned "1" then lines of the most abundant
isotope are taken, and so on.

The third field (string) is the line shape to be used in the line-by-line calculation for paths of the
specified gas. The following line shape options are provided:

“LORENTZ” the Lorentz line shape.

“DOPPLER” the Doppler line shape.

“VOIGT” the Voigt line shape using the Humlicek [1982] routine.

“VVH” the modified Van-Vleck Huber line shape [Clough et al., 1980].

“VOIGTCO2” the Voigt line shape modified for sub-Lorentzian $\text{CO}_2$ line wing behavior [Cousin
et al., 1985] and line coupling [Edwards and Strow, 1991].

“NEWSHAPE” for the user to supply their own line shape in subroutine new\_lineshape.f90.

“XSECTION” if the calculation is using cross-section data.

“AEROSOL” if the calculation is using aerosol data.

The fourth field (string) specifies if a continuum calculation is to be performed. Allowed values
are “CON” and “NOCON”.

The fifth field (integer) lists the line version parameters to distinguish between versions of duplicate
lines in the data file. This field will be called $lchose$ in the rest of this paragraph. If $lchose$ equals $m$,
then the most recent line versions up to and including lines with status number $m$ are used. Only
one version of any particular line will be used in the line-by-line calculation. For example, HITRUN
may be used to merge the HITRAN database (identified as having status 10) with line updates of a
particular gas (identified as having status 11). When HITRUN encounters a duplicate line, the line
with the lower status number will have its status number set equal to the negative of itself. Thus the
status number of a line on the HITRAN database that has been updated will be set to $-10$. If $lchose$
for this gas is equal to 11, GENRUN will then use lines that have a status number greater than or
equal to 10 and less than or equal to 11, or equal to $-11$. That is, the lines used have a status number
between 10 and $lchose$ inclusive, or equal to -$lchose$. This will not include the HITRAN lines with
status $-10$ that have been updated. However, if only HITRAN lines are required for the calculation
$lchose$ can be set to 10 and only lines with status numbers of $\pm 10$ will be used.

$\$LINE\_CUTOFF\_WIDE$ (real) - If positive, reject lines in the wide mesh calculation with path-
adjusted intensity less than this.

$\$LINE\_CUTOFF\_FINE$ (real) - If positive, reject lines in the fine mesh calculation with path-
adjusted intensity less than this.

$\$LINE\_MIXING$ This keyword is not mandatory and indicates that line coupling should be in-
cluded where appropriate. Data is currently available for the $\text{CO}_2 Q$-branches at 617, 667, 720, 740,
and 791 cm$^{-1}$, and is based on the $\text{CO}_2$ line parameters in file $\text{co2\_mix\_HT2012.asc}$. In using HITRUN
to create a line data file for line coupling, the lines in $\text{co2\_mix\_HT2012.asc}$ should be assigned the
highest status number. The carbon dioxide record in GAS\_TABLE should have its fifth field ($lchose$
see above) set equal to this status number so the required lines are selected. The VOIGTCO2 line
shape should be used for the lineshape parameter. In any computation with line coupling it is ES-
SENTIAL that the spectral range of the line-by-line calculation include all lines of the band for which
coupling parameters have been calculated. This is to satisfy the line strength and coupling parameter
sum rules [Strow and Reuter, 1988].
**XSCFIL**

This block is not mandatory. It includes the input necessary to define an absorption calculation for molecules for which cross-section data files are used.

$PATH_TO_XSFIL$ (string) - The path to the directory containing the HITRAN cross-section data (include a trailing ‘/’).

$NUMBER_OF_GASES$ (integer) - The number of gases for which cross-sections should be read.

$MOLECULE_IDS$ (integer) - List of molecular ID’s of the gases for which cross-sections are to be read from the file.

**MIXFIL**

This block defines the mixed path calculation. It is mandatory when MODE is PATH. The mixed paths are calculated internally (and this block is omitted) when MODE is NADIR, LIMB, FLUX, or CELL.

$NUMBER_MIXPATHS$ (integer) - The number of mixed paths, mandatory if the mixing table is explicitly listed in this block, in which case the keyword MIXING_TABLE must also appear.

$MIXPATH_FILE_NAME$ (string) - Mandatory if the mixing table is read from an external file. It is the name of the file and the file format is identical to the mixing table format used explicitly in this block. In this case the keyword MIXING_TABLE is not included.

Either $NUMBER_MIXPATHS$ or $MIXPATH_FILE_NAME$ is mandatory.

$MIXING_TABLE$ (real) - Flags the mixing table when $NUMBER_MIXPATHS$ is specified. The table is listed following this keyword. The input fields can be up to 130 characters wide. The entries for a particular mixed path may run over several lines of the input file, and input for a new mixed path must begin a new line.

It is often the case when mixing many paths together that a whole string of zeros or some other number must be entered in the table. In this case, an alternative to explicitly typing the number $x$ repeatedly $n$ times is to type $RxTn$. For example, a line of input “0 0 0 0 0” could be written $R0T5$. This reduces the physical size of the mixing table and helps prevent input errors. The mixing table entries should be written either as integers or $F$ format real numbers.

**AERFIL**

This block is not mandatory. Use it to include sulfate ($H_2SO_4$) aerosol. An example aerosol calculation is given in Section 8. The aerosol model is discussed in Section 7.6. When using aerosol it must also be listed in the GAS_TABLE of block *GASFIL. Sulfate is the only aerosol currently included in GENLN3.

$AEROSOL_FILE_NAME$ (string) - Name of the aerosol file.

$NUMBER_AEROSOLS$ (integer) - Number of aerosols to read from the file.

$AEROSOL_IDS$ (integer) - The ID’s of aerosols to be read.

$NORMALIZATION_WN$ (real) - Normalization wavenumber.

**RADNCE**

When MODE equals PATH, this block is mandatory if a radiance calculation is needed. The user must supply a mixing table. The RADNCE block is not used when MODE is NADIR, LIMB, CELL, or FLUX. The syntax of this block has a structure similar to GENLN2.

$NUMBER_OF_RADIATING_ATMOSPHERES$ (integer) - Specifies the number of different radiance (that is, “radiating atmosphere”) calculations to be performed.

$MAXIMUM_NUMBER_OF_LAYERS_PER_ATMOSPHERE$ (integer) - Maximum number of atmosphere layers present.

$LAYER_TABLE$ - This keyword flags a series of record groups, with each group defining one of the radiating atmosphere calculations. Each group contains five (or fewer) records. The number of groups is equal to $NUMBER_OF_RADIATING_ATMOSPHERES$. Not all five records are required in a given group: see the following description. Each group is laid out as follows:

$IATM, IVIEW, IEMS, NLAY, LAYSP$

$LAYER_1, LAYER_2, ... LAYER_NLAY$

$TBDY, TINIT, EMSTY$
LEMSP
LAYEMS₁, LAYEMS₂, ...LAYEMSₙLAY

IATM (integer) is the atmosphere index.

IVIEW (integer) is the viewing parameter. This can take two values which determine the boundary condition to be used in the radiation transfer equation as discussed in Section 7.9. If IVIEW = 1 then the radiance at the inward boundary to the first layer is set equal to zero. This would be appropriate to a limb emission calculation. If IVIEW = 2 a radiating surface boundary condition is applied. This would be appropriate for a nadir sounding problem where the surface emission term is non-negligible.

IEMS (integer) is the layer emission parameter. If IEMS = 1 then a single optical depth is later specified for each layer and this is used to determine both the layer transmittance and emission, i.e. \( \psi(\nu)_l \) and \( \phi(\nu)_l \) in Equation [43] are identical. Setting IEMS = 2 specifies an emission calculation and two optical depths are required for each layer, one to determine the layer transmittance \( \psi(\nu)_l \), and the other to determine the layer emission \( \phi(\nu)_l \).

NLAY (integer) specifies the number of layers for the atmosphere.

LAYSP (integer) indicates if the set of indices that follow (LAYER) for specifying the layer optical depth for the transmittance calculation \( \psi(\nu)_l \) (and emission calculation if IEMS = 1) refer to path numbers (LAYSP = 1) or mixed path numbers (LAYSP = 2).

LAYER (integer) is a list of NLAY indices referring to the path numbers (LAYSP = 1) or mixed path numbers (LAYSP = 2) whose optical depth are to be used to define the optical depths \( \psi(\nu)_l \) of the layers for the layer transmittance calculation. The indices defining each layer should be listed in the direction of radiation travel through the atmosphere.

If IVIEW = 2 then the parameters defining the radiating boundary surface come next. If IVIEW = 1 this section is absent.

TBĐY (real) is the temperature of the atmospheric boundary furthest away from the reflecting surface. For example in the case of a nadir viewing satellite, TBĐY = 2.96 K the temperature of cold space and the effective top of the atmosphere. This corresponds to the quantity \( T_b \) in Equation [40].

TINIT (real) is the boundary surface temperature corresponding to \( T_s \) in Equation [40].

EMSTY (real) is the surface emittance corresponding to \( \epsilon \) in Equation [40].

If IEMS = 2 then a different set of optical depths \( \phi(\nu)_l \) in Equation [43] are required to define the layer emission. If IEMS = 1 this section is absent.

LEMSP (integer) indicates if the set of indices that follow (LAYEMS) for specifying the layer optical depth \( \phi(\nu)_l \) for the emission calculation refer to path numbers, (LEMSP = 1) or mixed path numbers (LEMSP = 2).

LAYEMS (integer) is a list of NLAY indices referring to the path numbers (LEMSP = 1) or mixed path numbers (LEMSP = 2) whose optical depths are to be used to define the optical depths \( \phi(\nu)_l \) of the layers for the layer emission calculation. The indices defining each layer should be listed in the direction of radiation travel through the atmosphere.

*OUTPUT

This block is mandatory. Numerous keywords can be set to control the written output. Not all keyword combinations are allowed; this is calculation-dependent. GENLN3 will attempt to exit smoothly and provide useful diagnostic messages that flag incorrect combinations.

$OUTPUT_FILE_NAME (string) is the name of the NetCDF file containing the calculation results.

The following keywords are used when MODE is NADIR, LIMB, FLUX, or CELL:

$TRANSMITTANCE - If present, output transmittance spectra.

$OPTICAL_DEPTH - If present, output optical depth spectra.

$RADIANCE - If present, output radiance spectra.

$RADIANCE_COMPONENTS - If present, output individual radiance contributions that sum to the total radiance.

$GAS_CONTRIBUTIONS - If present, output spectra corresponding to each individual gas.

$FINE - If present, output spectra on the fine mesh.
$ALLLAYERS - If present, include spectra on all layers rather than only the boundary.
$WIDEMESH AVERAGE - If present, output spectra averaged over the wide mesh intervals

The following keywords are used when MODE is PATH. In this case the OUTPUT block syntax
has a structure similar to GENLN2.

$RADNCEOUTPUT - When MODE equals PATH, specifies that radiances defined in the *RAD-
NCE block will be output.
$NUMBEROFRADNCEDESCRIPTIONS - Used with RADNCEOUTPUT. The number of
radiance spectra to be output. These are described in $RADNCEOUTPUTTABLE.
$RADNCEOUTPUTTABLE - Used with RADNCEOUTPUT. This keyword flags a series of
record groups, with each group defining a particular output selection. The number of groups is equal
to NUMBEROFRADNCEDESCRIPTIONS. Each group contains three (or fewer) records: see the
following description. Each group is laid out as follows:

IDAT
IATM, NP
IOPGR1, IOPGR2,...IOPGRNP

IDAT (integer) is an output selection parameter with eight values:
1 for the path point transmittance spectra;
2 for the path integrated transmittance spectra;
3 for the mixed path point transmittance spectra;
4 for the mixed path integrated transmittance spectra;
5 for the radiating atmosphere layer point transmittance spectra;
6 for the radiating atmosphere layer integrated transmittance spectra;
7 for the radiating atmosphere layer point radiance spectra;
8 for the radiating atmosphere layer integrated radiance spectrum.
IATM (integer) specifies the relevant atmosphere number defined in *RADNCE (radiance calcu-
lution number) when IDAT > 4. If IDAT < 4 then IATM is absent. Setting IATM < 0 results in
spectra for all atmospheres being written.
NP (integer) specifies the number of paths, mixed paths or layers to be written. If NP < 0 then
all are written.
IOPGR (integer) is the list of NP (if NP > 0) path, mixed path, or layer numbers to be used.
IOPGR is absent if NP < 0.

*ENDINP
Mandatory. Marks the end of the input file.
8 Example Calculations

8.1 Example 1: Nadir calculation using the NADIR keyword

The following discussion applies in general form to all Examples discussed in this Section. Only brief remarks are included with Examples 2 through 7, which proceed similarly.

To set up GENLN3 for Example 1, the first step is to run the csh script `link_to_ex1_NADIR`. This will link the proper HITRUN and GENLN3 input files to their generic names `genln3` input and `HITRUN_input`. The script also links several IDL plotting codes to generic names. Using symbolic links with generic names makes many of the execution commands identical across all examples, which simplifies execution and avoids the need to keep track of the many different files names arising in each example. The plotting codes illustrate how to read and display some of the NetCDF output produced by GENLN3. NetCDF files can be examined directly using the `ndump` utility:

To look at the header: `ndump -h output.ncdf`
To look at the values of an output variable: `ndump -v variable_name output.ncdf`
To dump the entire file to ASCII: `ndump output.ncdf`

The links established by `link_to_ex1_NADIR` are the following:

\[\begin{align*}
\text{HITRUN\_input} & \rightarrow \text{HITRUN\_ip\_475_1700\_HT2012\_WITH\_CO2\_LINMIX.dat} \\
\text{genln3\_input} & \rightarrow \text{ex1\_genln3\_ip\_NADIR\_HT2012\_format.dat} \\
\text{plot\_data\_radiances\_gas\_contributions} & \rightarrow \text{ex1\_plotdata\_NADIR\_radiances\_gas\_contributions} \\
\text{plot\_data\_radiances} & \rightarrow \text{ex1\_plotdata\_NADIR\_radiances} \\
\text{plot\_data} & \rightarrow \text{ex1\_plotdata\_NADIR} \\
\end{align*}\]

Next, `hitrun` is executed to create the subsetted HITRAN binary data file used by GENLN3. Following this, GENLN3 is executed with the command `genrun`; the ASCII summary file `genln3` ascii summary.out and the NetCDF output are produced. The name of the NetCDF output file is located in `genln3` input.

\[\begin{align*}
\text{link_to_g3\_tech\_note\_example\_1\_NADIR} \\
\text{hitrun} \\
\text{genrun} \\
\end{align*}\]

The IDL codes (suffix `.pro`) produce postscript output which can be displayed using, for example, the UNIX utility `ghostview`:

\[\begin{align*}
\text{idl} \\
\text{>plot\_data} \\
\text{>exit} \\
\text{ghostview idl\_ex1\_plot\_data\_NADIR.ps} \\
\end{align*}\]

The IDL codes `plot\_data\_radiances.pro` and `plot\_data\_radiances\_gas\_contributions.pro` are run similarly.

For consistency checks some pre-computed reference output files are included with the software distribution. Depending on the specific example, the reference output may be in Postscript and/or NetCDF format. The reference filenames have the form `*.REF.gz` and are compressed with `gzip`. We mention again that our use of IDL for post-processing analysis and display is simply a user option.

Each example given below includes a listing of the necessary HITRUN and GENLN3 input files, as well as one or more plots of the calculation results. Sometimes the input files contain blocks or keywords that are commented out (using `"!"`). Rather than “polish” the input files, these unused sections are deliberately retained to highlight how a user might apply the commenting technique, and are a better reflection of how productive work often gets done in practice. Retaining unused sections is also a
8.1.1 Example 1: HITRUN Input File

```
* TITLES
$ TITLE :: 'HT2012 + CO2 line mixing 475_1700 wn'

* LINDAT
$ NUMBER_OF_FILES :: 2
$ FILE_TABLE
10, 'hitran2012.par'
11, 'co2_mix_HT2012.asc'

* RANGES
$ LOWER_WN :: 475.
$ UPPER_WN :: 1700.

* HITOUT
$ HITLIN_OUTPUT_FILE :: 'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'
```

8.1.2 Example 1: GENRUN Input File

```
* TITLES
$ TITLE : Overall title : 'ex1 NADIR HT2012'

* DEFGRD
$ MINIMUM_WAVENUMBER :: 825.
$ LOWER_INT_BOUND :: 850.
$ UPPER_INT_BOUND :: 1000.
$ MAXIMUM_WAVENUMBER :: 1025.
$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 100.
$ NUM_PER_HALFWIDTH :: -1.

* GEOMET
$ MODE :: 'NADIR'
$ ATM_BOUND : H or P : 'H'
$ ATM_LOWER_BOUND :: 0.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 0.0
$ AZIMUTH :: 0.0
$ TEMP_UPPER_BOUND :: 2.96.
$ TEMP_SURFACE :: 293.2
$ EMISSIVITY_SURFACE :: 0.9889
$ SUN_ZENITH :: 0.0
```
* OUTPUT

$ OUTPUT_FILE_NAME :: 'ex1_genln3_op_NADIR.ncdf'

$ TRANSMITTANCE

$ OPTICAL_DEPTH

$ RADIANCE

$ RADIANCE_COMPONENTS

$ GAS_CONTRIBUTIONS

$ FINE

$ ALL_LAYERS

* GASFIL

$ LINE_MIXING

$ NUMBER_OF_FILES :: 1

$ LINE_CUTOFF_WIDE :: 0.0

$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME

'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'

$ NUMBER_OF_GASES

3

$ GAS_TABLE

1, 0, 'VOIGT', 'CON' , 10
2, 0, 'VOIGTCO2', 'CON' , 11
3, 0, 'VOIGT', 'NOCON' , 10

* PTHFIL

---------------

$ USER_PROFILE : 'user profile' or 'model profile' are mandatory !

$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'

$ FLAG_ADD_ON

$ ADD_ON_FILE_NAME :: 'glatm.dat'

$ ADD_ON_PROF_NUMBER :: 2

---------------

!$ MODEL_PROFILE : 'user profile' or 'model profile' are mandatory !

!$ MODPRO_FILE_NAME :: 'glatm.dat'

!$ PROFILE_NUMBER :: 6

---------------

!$ REFRACITION

---------------

$ USER_LAYERS
$ LAYERBOUND : H or P: 'H'
$ LAYERNUMBER : 24
$ SUB_LAYERNUMBER : 10

$ LAYER_TABLE :
1 0.000 1.100
2 1.100 2.200
3 2.200 3.100
4 3.100 4.000
5 4.000 4.900
6 4.900 5.800
7 5.800 6.700
8 6.700 7.600
9 7.600 8.500
10 8.500 9.400
11 9.400 10.400
12 10.400 11.400
13 11.400 12.400
14 12.400 16.900
15 16.900 21.400
16 21.400 26.300
17 26.300 31.000
18 31.000 35.300
19 35.300 39.800
20 39.800 44.700
21 44.700 60.400
22 60.400 65.400
23 65.400 71.400
24 71.400 80.000

----------

$ DEFAULT LAYERS : 'mandatory or user layers'

$ SUB_LAYERNUMBER : 10

$ MAX_VAR_VOIGT_HW : (should be between 1 and 2) : 2.0
$ MAX TEMP DIFF_BOT : (K) : 5.0
$ MAX TEMP DIFF_TOA : (K) : 30.0

---------------------------------------------------------------------

* XSCFIL

$ PATH TO XSFILES : trailing '/': 'HIT2012/IR-XSect/Uncompressed-files/

$ NUMBER OF GASES : 1
$ MOLECULE IDS : -number of gases- values : 52

---------------------------------------------------------------------

!* MIXFIL

$ MIXPATH_FILE_NAME : or mixpath filename: 28

$ NUMBER OF MIXPATHS : or mixpath filename: 28

$ MIXING_TABLE :
1 R0T0 1 R0T23 R0T0 1 R0T23 R0T0 1 R0T23
2 R0T1 1 R0T22 R0T1 1 R0T22 R0T1 1 R0T22
3 R0T2 1 R0T21 R0T2 1 R0T21 R0T2 1 R0T21
4 R0T3 1 R0T20 R0T3 1 R0T20 R0T3 1 R0T20
5 R0T4 1 R0T19 R0T4 1 R0T19 R0T4 1 R0T19
6 R0T5 1 R0T18 R0T5 1 R0T18 R0T5 1 R0T18
7 R0T6 1 R0T17 R0T6 1 R0T17 R0T6 1 R0T17
8 R0T7 1 R0T16 R0T7 1 R0T16 R0T7 1 R0T16
9 Rot8 1 Rot15 Rot8 1 Rot15 Rot8 1 Rot15 Rot8 1 Rot15
10 Rot9 1 Rot14 Rot9 1 Rot14 Rot9 1 Rot14 Rot9 1 Rot14
11 Rot10 1 Rot13 Rot10 1 Rot13 Rot10 1 Rot13 Rot10 1 Rot13
12 Rot11 1 Rot12 Rot11 1 Rot12 Rot11 1 Rot12 Rot11 1 Rot12
13 Rot12 1 Rot11 Rot12 1 Rot11 Rot12 1 Rot11 Rot12 1 Rot11
14 Rot13 1 Rot10 Rot13 1 Rot10 Rot13 1 Rot10 Rot13 1 Rot10
15 Rot14 1 Rot9 Rot14 1 Rot9 Rot14 1 Rot9 Rot14 1 Rot9
16 Rot15 1 Rot8 Rot15 1 Rot8 Rot15 1 Rot8 Rot15 1 Rot8
17 Rot16 1 Rot7 Rot16 1 Rot7 Rot16 1 Rot7 Rot16 1 Rot7
18 Rot17 1 Rot6 Rot17 1 Rot6 Rot17 1 Rot6 Rot17 1 Rot6
19 Rot18 1 Rot5 Rot18 1 Rot5 Rot18 1 Rot5 Rot18 1 Rot5
20 Rot19 1 Rot4 Rot19 1 Rot4 Rot19 1 Rot4 Rot19 1 Rot4
21 Rot20 1 Rot3 Rot20 1 Rot3 Rot20 1 Rot3 Rot20 1 Rot3
22 Rot21 1 Rot2 Rot21 1 Rot2 Rot21 1 Rot2 Rot21 1 Rot2
23 Rot22 1 Rot1 Rot22 1 Rot1 Rot22 1 Rot1 Rot22 1 Rot1
24 Rot23 1 Rot0 Rot23 1 Rot0 Rot23 1 Rot0 Rot23 1 Rot0
25 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24
26 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24
27 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24
28 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24 Rot24

* AERFIL

!* AEROSOL_FILE_NAME :: ''
!* NUMBER_AEROSOLS :: 0
!* AEROSOL_IDS : -number aerosols- values : 0
!* NORMALIZATION_WN : -number aerosols- values: 0.0

* ENDINP
8.1.3 Example 1: Output

Figure 6: Example 1 (Nadir calculation via NADIR keyword): Individual transmittance spectra for $H_2O$, $CO_2$, $O_3$, and $CFC12$. Also the total transmitance of all gases calculated two ways, and their (small) difference.
Figure 7: Example 1 (Nadir calculation via NADIR keyword): TOA total nadir radiance due to $H_2O$, $CO_2$, $O_3$, and $CFC12$ along with solar, surface, and atmospheric contributions. Verification that the sum of the radiance components is equal to the independently-reported total radiance. Nadir radiance spectra from TOA down to selected levels.
Figure 8: Example 1 (Nadir calculation via NADIR keyword): TOA radiance contributions by $H_2O$, $CO_2$, $O_3$, and $CFC12$ individually. Also, the total radiance calculated two ways, and their (small) difference.

### 8.2 Example 2: Nadir calculation using the PATH keyword

```
link_to_g3_tech_note_example_2_PATH
hitrun
genrun
idl
>compile plot_data
>plot_data
>exit
ghostview idl_ex2_plot_data_PATH.ps
```

#### 8.2.1 Example 2: HITRUN Input File

Same as Example 1.
8.2.2 Example 2: GENRUN Input File

* TITLES

$ TITLE : Overall title : 'ex1 PATH HT2012'

* DEFGRD

$ MINIMUM_WAVENUMBER :: 825.
$ LOWER_INT_BOUND :: 850.
$ UPPER_INT_BOUND :: 1000.
$ MAXIMUM_WAVENUMBER :: 1025.
$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 100
$ NUM_PER_HALFWIDTH :: -1

* GEOMET

$ MODE :: 'PATH'
$ ATM_BOUND : H or P : 'H'
$ ATMLOWERBOUND :: 0.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 0.0
$ AZIMUTH :: 0.0
$ TEMP_UPPER_BOUND :: 2.96
$ TEMP_SURFACE :: 293.2
$ EMISSIVITY_SURFACE :: 0.9889
$ SUN_ZENITH :: 0.0

* GASFIL

$ LINE_MIXING

$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME
'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'

$ NUMBER_OF_GASES
3

$ GAS_TABLE
1, 0, 'VOIGT', 'CON', 10
2, 0, 'VOIGTCO2', 'CON', 11
3, 0, 'VOIGT', 'NOCON', 10

* XSCFIL
$ PATH_TO_XSFILES : incl trailing'/' : 'HIT2012/IR-XSect/Uncompressed-files/'

$ NUMBER_OF_GASES :: 1
$ MOLECULE_IDS : -number of gases- values : 52

* PTHFIL

$ USER_PROFILE : 'user profile' or 'model profile' are mandatory !
$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'
$ FLAG_ADD_ON
$ ADD_ON_FILE_NAME :: 'glatm.dat'
$ ADD_ON_PROF_NUMBER :: 2

* MODEL_PROFILE : 'user profile' or 'model profile' are mandatory !
$ MODPRO_FILE_NAME :: 'glatm.dat'
$ PROFILE_NUMBER :: 6

* REFRACITION

$ USER_LAYERS

$ LAYER_SOUND : H or P: 'H'
$ LAYER_NUMBER :: 24
$ SUB_LAYER_NUMBER :: 10
$ LAYER_TABLE :
1 0.00 1.10
2 1.10 2.16
3 2.16 3.04
4 3.04 3.92
5 3.92 4.82
6 4.82 5.74
7 5.74 6.64
8 6.64 7.52
9 7.52 8.42
10 8.42 9.34
11 9.34 10.28
12 10.28 11.24
13 11.24 12.22
14 12.22 16.72
15 16.72 21.16
16 21.16 25.94
17 25.94 30.80
18 30.80 35.12
19 35.12 39.62
20 39.62 44.54
21 44.54 61.38
22 61.38 67.18
23 67.18 78.10
24 78.10 80.00

* MIXFIL

48
$ NUMBER_MIXPATHS : or mixpath filename: 28

!$ MIXPATH_FILE_NAME : or number mixpaths: ''

$ MIXING_TABLE :
1  R0T0  1 R0T23  R0T0  1 R0T23  R0T0  1 R0T23
2  R0T1  1 R0T22  R0T1  1 R0T22  R0T1  1 R0T22
3  R0T2  1 R0T21  R0T2  1 R0T21  R0T2  1 R0T21
4  R0T3  1 R0T20  R0T3  1 R0T20  R0T3  1 R0T20
5  R0T4  1 R0T19  R0T4  1 R0T19  R0T4  1 R0T19
6  R0T5  1 R0T18  R0T5  1 R0T18  R0T5  1 R0T18
7  R0T6  1 R0T17  R0T6  1 R0T17  R0T6  1 R0T17
8  R0T7  1 R0T16  R0T7  1 R0T16  R0T7  1 R0T16
9  R0T8  1 R0T15  R0T8  1 R0T15  R0T8  1 R0T15
10 R0T9  1 R0T14  R0T9  1 R0T14  R0T9  1 R0T14
11 R0T10 1 R0T13 R0T10 1 R0T13 R0T10 1 R0T13
12 R0T11 1 R0T12 R0T11 1 R0T12 R0T11 1 R0T12
13 R0T12 1 R0T11 R0T12 1 R0T11 R0T12 1 R0T11
14 R0T13 1 R0T10 R0T13 1 R0T10 R0T13 1 R0T10
15 R0T14 1 R0T9  R0T14 1 R0T9  R0T14 1 R0T9
16 R0T15 1 R0T8  R0T15 1 R0T8  R0T15 1 R0T8
17 R0T16 1 R0T7  R0T16 1 R0T7  R0T16 1 R0T7
18 R0T17 1 R0T6  R0T17 1 R0T6  R0T17 1 R0T6
19 R0T18 1 R0T5  R0T18 1 R0T5  R0T18 1 R0T5
20 R0T19 1 R0T4  R0T19 1 R0T4  R0T19 1 R0T4
21 R0T20 1 R0T3  R0T20 1 R0T3  R0T20 1 R0T3
22 R0T21 1 R0T2  R0T21 1 R0T2  R0T21 1 R0T2
23 R0T22 1 R0T1  R0T22 1 R0T1  R0T22 1 R0T1
24 R0T23 1 R0T0  R0T23 1 R0T0  R0T23 1 R0T0
25 R1T24  R0T24  R0T24  R0T24
26 R0T24  R1T24  R0T24  R0T24
27 R0T24  R0T24  R1T24  R0T24
28 R0T24  R0T24  R0T24  R1T24

---------------------------------------------------------------------
!* AERFIL

!$ AEROSOL_FILE_NAME :: ''

!$ NUMBER_AEROSOLS :: 0
!$ AEROSOL_IDS : -number aerosols- values : 0

!$ NORMALIZATION_WN :-number aerosols- values: 0.0

---------------------------------------------------------------------
* RADNCE

$ NUMBER_OF_RADIANATING_ATMOSPHERES :: 3

$ MAXIMUM_NUMBER_OF_LAYERS_PER_ATMOSPHERE :: 24

$ LAYER_TABLE
1 2 1 24 2
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
2.96 293.2 0.9889
2 1 19 2
6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
2.96 265.0 1.0
3 1 13 2
12 13 14 15 16 17 18 19 20 21 22 23 24
2.96 230.0 1.0

---------------------------------------------------------------------
* OUTPUT

49
$ OUTPUT_FILE_NAME :: 'ex1_genln3_op_PATH.ncdf'

$ RADNCE_OUTPUT

$ NUMBER_OF_RADNCE_DESCRIPTIONS :: 13

$ RADNCE_OUTPUT_TABLE
3
4
25 26 27 28
7
1 1
24
7
2 1
19
7
3 1
13
8
1 1
24
8
2 1
19
8
3 1
13
5
1 1
24
5
2 1
19
5
3 1
13
6
1 1
24
6
2 1
19
6
3 1
13

-----------------------------------------------
* ENDP
8.2.3 Example 2: Output

Figure 9: Example 2 (Nadir calculation via PATH keyword): Individual TOA transmittance spectra for \( H_2O \), \( CO_2 \), \( O_3 \), and \( CFC12 \) computed using PATH (first column) and comparison with spectra obtained using NADIR (second column). Differences between the two calculations (third column) are small.
Figure 10: Example 2 (Nadir calculation via PATH keyword): TOA radiance spectra due to $H_2O$, $CO_2$, $O_3$, and $CFC12$ for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated and plotted on the fine mesh grid.
Figure 11: Example 2 (Nadir calculation via PATH keyword): TOA radiance spectra due to $H_2O$, $CO_2$, $O_3$, and $CFC12$ for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated on the fine mesh but plotted on the wide mesh integrated grid.
Figure 12: Example 2 (Nadir calculation via PATH keyword): TOA transmittance spectra due to $H_2O$, $CO_2$, $O_3$, and $CFC12$ for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated and plotted on the fine mesh grid.
Figure 13: Example 2 (Nadir calculation via PATH keyword): TOA transmittance spectra due to $H_2O$, $CO_2$, $O_3$, and $CFC12$ for a clear sky atmosphere bounded below by the surface (black), along with corresponding spectra for regions bounded below by opaque cloud layers at 5 km (red) and 10 km (blue). Spectra calculated on the fine mesh but plotted on the wide mesh integrated grid.

8.3 Example 3: Limb calculation using the LIMB keyword

8.3.1 Example 3: HITRUN Input File

Same as Example 1.

8.3.2 Example 3: GENRUN Input File

```
* TITLES
$ TITLE : Overall title : 'ex2 LIMB HT2012'

* DEFGRD
$ MINIMUM_WAVENUMBER :: 693.
```
$ LOWER_INT_BOUND :: 718.
$ UPPER_INT_BOUND :: 722.
$ MAXIMUM_WAVENUMBER :: 747.
$ WIDE_INTERVAL_SPAC :: 1.

$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 40
$ NUM_PER_HALFWIDTH :: -1

* GEOMET

$ MODE :: 'LIMB'
$ ATM_BOUND : H or P: 'H'

$ ATM_LOWER_BOUND :: 30.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 90.
$ AZIMUTH :: 0.0

$ TEMP_UPPER_BOUND :: 2.96

* OUTPUT

$ OUTPUT_FILE_NAME :: 'ex2_genln3_op_LIMB.ncdf'

$ RADIANCE
$ TRANSMITTANCE
$ OPTICAL_DEPTH

$ GAS_CONTRIBUTIONS
$ RADIANCE_COMPONENTS

$ FINE

$ ALL_LAYERS

* GASFIL

$ LINE_MIXING

$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME
'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'

$ NUMBER_OF_GASES
2

$ GAS_TABLE
2, 0, 'VOIGTCO2', 'CON' , 11
3, 0, 'VOIGT', 'NOCON', 10

* PTHFIL

$ USER_PROFILE : 'user profile' or 'model profile' are mandatory!

$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'
$ MODEL_PROFILE : 'user profile' or 'model profile' are mandatory!

$ MODPRO_FILE_NAME :: 'glatm.dat'
$ PROFILE_NUMBER :: 6

$ REFRACTION

$ USER_LAYERS

$ LAYER_BOUND : H or P: 'H'
$ LAYER_NUMBER :: 20
$ SUB_LAYER_NUMBER :: 10

$ LAYER_TABLE :
1 30.0 30.5
2 30.5 31.0
3 31.0 32.0
4 32.0 33.0
5 33.0 34.0
6 34.0 35.0
7 35.0 36.0
8 36.0 37.0
9 37.0 38.0
10 38.0 40.0
11 40.0 42.0
12 42.0 44.0
13 44.0 46.0
14 46.0 48.0
15 48.0 50.0
16 50.0 55.0
17 55.0 60.0
18 60.0 65.0
19 65.0 70.0
20 70.0 80.0

* XSCFIL

$ PATH_TO_XSFIL : include trailing '/' !: '/MOPITT/data/gfrancis/HIT2000/IR-XSect/

$ NUMBER_OF_GASES :: 1
$ MOLECULE_IDS : -number of gases- values : 52

* MIXFIL

$ NUMBER_MIXPATHS : or mixpath filename: 20
$ MIXPATH_FILE_NAME : or number mixpaths: ''

$ MIXING_TABLE :
1 ROT0 1 ROT19 ROT0 1 ROT19
2 ROT1 1 ROT18 ROT1 1 ROT18
3 ROT2 1 ROT17 ROT2 1 ROT17
4 ROT3 1 ROT16 ROT3 1 ROT16
5 ROT4 1 ROT15 ROT4 1 ROT15
6 ROT5 1 ROT14 ROT5 1 ROT14
7 ROT6 1 ROT13 ROT6 1 ROT13
8 ROT7 1 ROT12 ROT7 1 ROT12
9 ROT8 1 ROT11 ROT8 1 ROT11
10 ROT9 1 ROT10 ROT9 1 ROT10
11 ROT10 1 ROT9 ROT10 1 ROT9
12 ROT11 1 ROT8 ROT11 1 ROT8
13 ROT12 1 ROT7 ROT12 1 ROT7
14 ROT13 1 ROT6 ROT13 1 ROT6
15 ROT14 1 ROT5 ROT14 1 ROT5
16 ROT15 1 ROT4 ROT15 1 ROT4
17 ROT16 1 ROT3 ROT16 1 ROT3
18 ROT17 1 ROT2 ROT17 1 ROT2
19 ROT18 1 ROT1 ROT18 1 ROT1
20 ROT19 1 ROT0 ROT19 1 ROT0

---------------------------------------------------------------------
!* AERFIL

!*$ AEROSOL_FILE_NAME :: ''
!*$ NUMBER_AEROSOLS :: 0
!*$ AEROSOL_IDS : -number aerosols- values : 0

!*$ NORMALIZATION_WN :-number aerosols- values: 0.0

---------------------------------------------------------------------
!* ENDINP
8.3.3 Example 3: Output

Figure 14: Example 3 (Limb calculation via LIMB keyword): Total limb radiance and individual contributions by CO$_2$ and O$_3$ for a 30km tangent height. Total limb transmittance and individual contributions by CO$_2$ and O$_3$. Limb transmittance for levels 30, 20, 10, and 0, the latter lying near TOA. Transmittance and radiance differences for two calculation techniques are small.

8.4 Example 4: Limb calculation using the PATH keyword

8.4.1 Example 4: HITRUN Input File

Same as Example 1.

8.4.2 Example 4: GENRUN Input File

* TITLES

$ TITLE : Overall title : 'Limb View Calc GENLN3 via PATH'
* DEFGRD

$ MINIMUM_WAVENUMBER :: 693.
$ LOWER_INT_BOUND :: 718.
$ UPPER_INT_BOUND :: 722.
$ MAXIMUM_WAVENUMBER :: 747.
$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 40
$ NUM_PER_HALFWIDTH :: -1

* GEOMET

$ MODE :: 'PATH'
$ ATM_BOUND : H or P: 'H'
$ ATM_LOWER_BOUND :: 30.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 90.
$ AZIMUTH :: 0.0
$ TEMP_UPPER_BOUND :: 2.96
$ TEMP_SURFACE :: 293.2
$ EMISSIVITY_SURFACE :: 1.0
$ SUN_ZENITH :: 0.0

* GASFIL

$ LINE_MIXING
$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0
$ GAS_FILE_NAME
 'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'
$ NUMBER_OF_GASES
2
$ GAS_TABLE
2, 0, 'VOIGTCO2', 'CON' , 11
3, 0, 'VOIGT', 'NOCON' , 10

* PTHFIL

--

!$ USER_PROFILE : 'user profile' or 'model profile' are mandatory !

!$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'

!$ FLAG_ADD_ON
!$ ADD_ON_FILE_NAME :: 'glatm.dat'

60
!$ ADD_ON_PROF_NUMBER :: 2

---------------

$ MODEL_PROFILE : 'user profile' or 'model profile' are mandatory!

$ MODPRO_FILE_NAME :: 'glatm.dat'
$ PROFILE_NUMBER :: 6

---------------

$ REFRACTION

---------------

$ USER_LAYERS

$ LAYER_BOUND : H or P: 'H'
$ LAYER_NUMBER :: 20
$ SUB_LAYER_NUMBER :: 10

$ LAYER_TABLE :
1 30.0 30.5
2 30.5 31.0
3 31.0 32.0
4 32.0 33.0
5 33.0 34.0
6 34.0 35.0
7 35.0 36.0
8 36.0 37.0
9 37.0 38.0
10 38.0 40.0
11 40.0 42.0
12 42.0 44.0
13 44.0 46.0
14 46.0 48.0
15 48.0 50.0
16 50.0 55.0
17 55.0 60.0
18 60.0 65.0
19 65.0 70.0
20 70.0 80.0

---------------

!$ XSCFIL

!$ PATH_TO_XSFILES : include trailing '/': '/MOPITT/data/gfrancis/HIT2000/IR-XSect/

!$ NUMBER_OF_GASES :: 1
!$ MOLECULE_IDS : -number of gases- values : 52

* MIXFIL

$ NUMBER_MIXPATHS : or mixpath filename: 20

!$ MIXPATH_FILE_NAME : or number mixpaths: ''

$ MIXING_TABLE :
1 ROT0 1 ROT19 ROT0 1 ROT19
2 ROT1 1 ROT18 ROT1 1 ROT18
3 ROT2 1 ROT17 ROT2 1 ROT17
4 ROT3 1 ROT16 ROT3 1 ROT16
* RADNCE

$ NUMBER_OF_RADIATING_ATMOSPHERES :: 3

$ MAXIMUM_NUMBER_OF_LAYERS_PER_ATMOSPHERE :: 40

$ LAYER_TABLE
  1 1 2 40 2
  20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
1
  20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
2 1 2 40 2
  20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
1
  40 39 38 37 36 35 34 33 32 31 30 29 28 27 26 25 24 23 22 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35
  36 37 38 39 40
3 1 1 40 2
  20 19 18 17 16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

* OUTPUT

$ OUTPUT_FILE_NAME :: 'ex2_genln3_op_PATH.ncdf'

$ RADNCE_OUTPUT

$ NUMBER_OF_RADNCE_DESCRIPTIONS :: 2

$ RADNCE_OUTPUT_TABLE
  5
  -1 1
  40
  7
   -1 1
  40

* AERFIL

!$ AEROSOL_FILE_NAME :: ''

!$ NUMBER_AEROSOLS :: 0
!$ AEROSOL_IDS : -number aerosols- values : 0

!$ NORMALIZATION_WN :: -number aerosols- values: 0.0

* ENDINP

62
8.4.3 Example 4: Output

Figure 15: Example 4 (Limb calculation via PATH keyword): Total limb transmittance due to $CO_2$ and $O_3$ for a 30 km tangent height computed using PATH, and comparison with transmittance obtained using LIMB.
Figure 16: Example 4 (Limb calculation via PATH keyword): Individual limb radiance contributions from CO\textsubscript{2} and O\textsubscript{3} for a 30 \textit{km} tangent height.

8.5 Example 5: Gas cell transmittance calculation using the CELL keyword

\texttt{link_to_g3\_tech\_note\_example\_5\_CELL}

8.5.1 Example 5: HITRUN Input File

```
$TITLE :: 'HT2012 + CO2 line mixing 1700-2400 wn'

$LINDAT
$NUMBER_OF_FILES :: 2
$FILE_TABLE
10, 'hitran2012.par'
11, 'co2_mix_HT2012.asc'

$RANGES
$LOWER_WN :: 1700.
$UPPER_WN :: 2400.
```
8.5.2 Example 5: GENRUN Input File

--- Titles

$ TITLE : Overall title : 'MOPITT CO CELL CALC'

--- DefGrd

$ MINIMUM_WAVENUMBER :: 1935.
$ LOWER_INT_BOUND :: 1960.
$ UPPER_INT_BOUND :: 2352.
$ MAXIMUM_WAVENUMBER :: 2377.
$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 400
$ NUM_PER_HALFWIDTH :: -1

--- Geomet

$ MODE :: 'CELL'
$ CELL_FILE_NAME :: 'ct.path'

--- Output

$ OUTPUT_FILE_NAME :: 'ex0_genln3_op_CELL.ncdf'

--- Transmittance

$ Fine

--- GasFil

$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME
'hitlin_op_1700_2400_HT2012_WITH_CO2_LINMIX.bin'
$ NUMBER_OF_GASES
1
$ GAS_TABLE
5, 0, 'VOIGT', 'NOCON', 10 : for MODE=CELL, all params are ignored except gasid, others are read in CELL_FILE_NAME :

--- Endinp
8.5.3 Example 5: Input file \textit{ct.path}

\begin{verbatim}
2
1 PATH #1: pmc 50mb high-pressure state
   5 0 1.90848e-09 315.10 315.10 315.10 0.04934616334 0.04934616334 0.04934616334
       'VOIGT' 'NOCON'

1 PATH #2: pmc 28mb low-pressure state
   5 0 1.20868e-09 278.62 278.62 278.62 0.02763385147 0.02763385147 0.02763385147
       'VOIGT' 'NOCON'
\end{verbatim}

8.5.4 Example 5: Output

\begin{itemize}
\item Two-State PMR: Difference Transmittance via CELL Calculation
\item Two-State PMR: Average Transmittance via CELL Calculation
\end{itemize}

Figure 17: Example 5 (Cell transmittance via CELL keyword): Segment of the Average and Difference transmittance spectra for a two-state model of a pressure-modulated radiometer (PMR). The spectral interval plotted lies in the $0-1 \ CO$ fundamental band. Cell calculations similar to these enable global remote sensing of tropospheric $CO$ via gas correlation radiometry by the NASA EOS/MOPITT instrument on board the Terra spacecraft [Drummond et al., 2010].

8.6 Example 6: Flux calculation using the FLUX keyword

\textit{link_to_g3_tech_note_example_6_FLUX}
8.6.1 Example 6: HITRUN Input File

Same as Example 1.

8.6.2 Example 6: GENRUN Input File

```
* TITLES
$ TITLE : Overall title : 'ex1 FLUX'

* DEFGRD
! basic test
! O3 region
$ MINIMUM_WAVENUMBER :: 955.
$ LOWER_INT_BOUND :: 980.
$ UPPER_INT_BOUND :: 1180.
$ MAXIMUM_WAVENUMBER :: 1205.
$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 50
$ NUM_PER_HALFWIDTH :: -1

* GEOMET
$ MODE :: 'FLUX'
$ ATM_BOUND : H or P: 'H'

$ ATM_LOWER_BOUND :: 0.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 0.0
$ AZIMUTH :: 0.0
$ TEMP_UPPER_BOUND :: 2.96
$ TEMP_SURFACE :: 298.0
$ EMISSIVITY_SURFACE :: 0.98
$ SUN_ZENITH :: 0.0

* OUTPUT
$ OUTPUT_FILE_NAME :: 'ex1_genln3_op_FLUX.ncdf'

$ TRANSMITTANCE
$ RADIANCE

$ RADIANCE_COMPONENTS
$ GAS_CONTRIBUTIONS

$ FINE
$ ALL_LAYERS
$ WIDE_MESH_AVERAGE
```
* GASFIL

$ LINE_MIXING

$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME
'hitlin_op_475_1700_HT2012_WITH_CU2_LINMIX.bin'

$ NUMBER_OF_GASES
3

$ GAS_TABLE
1, 0, 'VOIGT', 'CON', 10
2, 0, 'VOI_GTCO2', 'CON', 10
3, 0, 'VOIGT', 'NOCON', 10

* PTHFIL

$ USER_PROFILE : 'user profile' or 'model profile' are mandatory!

$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'

$ FLAG_ADD_ON
$ ADD_ON_FILE_NAME :: 'glatm.dat'
$ ADD_ON_PROF_NUMBER :: 2

--------------

!$ MODEL_PROFILE : 'user profile' or 'model profile' are mandatory!

!$ MODPRO_FILE_NAME :: 'glatm.dat'
!$ PROFILE_NUMBER :: 6

--------------

!$ REFRACTION

--------------

!$ USER_LAYERS

!$ LAYER_BOUND : H or P: 'H'
!$ LAYER_NUMBER :: 20
!$ SUB_LAYER_NUMBER :: 10

!$ LAYER_TABLE :
1 30.0 30.5
2 30.5 31.0
3 31.0 32.0
4 32.0 33.0
5 33.0 34.0
6 34.0 35.0
7 35.0 36.0
8 36.0 37.0
9 37.0 38.0
10 38.0 40.0
11 40.0 42.0
$ DEFAULT_LAYERS : 'mandatory or user layers'

$ SUB_LAYER_NUMBER :: 10

$ MAX_VAR_VOIGT_HW : (should be between 1 and 2) : 2.0
$ MAX_TEMP_DIFF_BOT :(K): 5.0
$ MAX_TEMP_DIFF_TOA :(K): 30.0

* XSCFIL

$ PATH_TO_XSFILES : include '/': 'HIT2012/IR-XSect/Uncompressed-files/

$ NUMBER_OF_GASES :: 1
$ MOLECULE_IDS :: -number of gases- values : 52

*! MIXFIL

!* NUMBER_MIXPATHS : or mixpath filename: 28
!* MIXPATH_FILE_NAME : or number mixpaths: '

!* MIXING_TABLE :
1 ROT0 1 ROT23 ROT0 1 ROT23 ROT0 1 ROT23 1 ROT0 1 ROT23
2 ROT1 1 ROT22 ROT1 1 ROT22 ROT1 1 ROT22 1 ROT1 1 ROT22
3 ROT2 1 ROT21 ROT2 1 ROT21 ROT2 1 ROT21 1 ROT2 1 ROT21
4 ROT3 1 ROT20 ROT3 1 ROT20 ROT3 1 ROT20 1 ROT3 1 ROT20
5 ROT4 1 ROT19 ROT4 1 ROT19 ROT4 1 ROT19 1 ROT4 1 ROT19
6 ROT5 1 ROT18 ROT5 1 ROT18 ROT5 1 ROT18 1 ROT5 1 ROT18
7 ROT6 1 ROT17 ROT6 1 ROT17 ROT6 1 ROT17 1 ROT6 1 ROT17
8 ROT7 1 ROT16 ROT7 1 ROT16 ROT7 1 ROT16 1 ROT7 1 ROT16
9 ROT8 1 ROT15 ROT8 1 ROT15 ROT8 1 ROT15 1 ROT8 1 ROT15
10 ROT9 1 ROT14 ROT9 1 ROT14 ROT9 1 ROT14 1 ROT9 1 ROT14
11 ROT10 1 ROT13 ROT10 1 ROT13 ROT10 1 ROT13 1 ROT10 1 ROT13
12 ROT11 1 ROT12 ROT11 1 ROT12 ROT11 1 ROT12 1 ROT11 1 ROT12
13 ROT12 1 ROT11 ROT12 1 ROT11 ROT12 1 ROT11 1 ROT12 1 ROT11
14 ROT13 1 ROT10 ROT13 1 ROT10 ROT13 1 ROT10 1 ROT13 1 ROT10
15 ROT14 1 ROT9 ROT14 1 ROT9 ROT14 1 ROT9 1 ROT14 1 ROT9
16 ROT15 1 ROT8 ROT15 1 ROT8 ROT15 1 ROT8 1 ROT15 1 ROT8
17 ROT16 1 ROT7 ROT16 1 ROT7 ROT16 1 ROT7 1 ROT16 1 ROT7
18 ROT17 1 ROT6 ROT17 1 ROT6 ROT17 1 ROT6 1 ROT17 1 ROT6
19 ROT18 1 ROT5 ROT18 1 ROT5 ROT18 1 ROT5 1 ROT18 1 ROT5
20 ROT19 1 ROT4 ROT19 1 ROT4 ROT19 1 ROT4 1 ROT19 1 ROT4
21 ROT20 1 ROT3 ROT20 1 ROT3 ROT20 1 ROT3 1 ROT20 1 ROT3
22 ROT21 1 ROT2 ROT21 1 ROT2 ROT21 1 ROT2 1 ROT21 1 ROT2
23 ROT22 1 ROT1 ROT22 1 ROT1 ROT22 1 ROT1 1 ROT22 1 ROT1
24 ROT23 1 ROT0 ROT23 1 ROT0 ROT23 1 ROT0 1 ROT23 1 ROT0
25 R1T24 ROT24 R1T24 R2T4 R2T4 R2T4
26 R2T24 R1T24 R2T24 R2T4 R2T4 R2T4
27 R2T24 R2T24 R1T24 R1T4 R1T4 R1T4
28 R2T24 R2T24 R2T24 R1T24 R1T24 R1T24
8.6.3 Example 6: Output

Figure 18: Example 6 (Flux calculation via FLUX keyword): Upward, downward, and total flux as a function of altitude, together with the corresponding cooling rate, for the infrared wavenumber interval [980, 1180], which includes the strong 9.6 μm O₃ band. Gases used in this calculation are H₂O, CO₂, O₃, and CFC12.
8.7 Example 7: Radiance looking upward through atmosphere to space

Example 7: HITRUN Input File

Same as Example 1.

8.7.2 Example 7: GENRUN Input File

```plaintext
!-------------------------------------------------------------------------------
* TITLES
$ TITLE :: 'Example 1 zenith calc looking up GENLN3'
!-------------------------------------------------------------------------------
* GEOMET
$ MODE :: 'PATH'
$ ATM_BOUND : H or P: 'H'
$ ATM_LOWER_BOUND :: 0.
$ ATM_UPPER_BOUND :: 80.
$ VIEW_ZENITH :: 0.0
$ AZIMUTH :: 0.0
$ TEMP_UPPER_BOUND :: 2.96
$ TEMP_SURFACE : not used in this calc : 1.0
$ EMISSIVITY_SURFACE : not used in this calc : 0.0
$ SUN_ZENITH :: 0.0
!-------------------------------------------------------------------------------
* GASFIL
$ LINE_MIXING
$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0
$ GAS_FILE_NAME
  'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'
$ NUMBER_OF_GASES
  3

$ GAS_TABLE
  1, 0, 'VOIGT', 'CON', 10
  2, 0, 'VOIGTCO2', 'CON', 11
  3, 0, 'VOIGT', 'NOCON', 10

!-------------------------------------------------------------------------------
* XSCFIL
$ PATH_TO_XSFFILES : incl trailing'/' : 'HIT2012/IR-XSect/Uncompressed-files/'
$ NUMBER_OF_GASES :: 1
$ MOLECULE_IDS :: 52
!-------------------------------------------------------------------------------
```
* DEFINITION

$ MINIMUM_WAVENUMBER :: 825.
$ LOWER_INT_BOUND :: 850.
$ UPPER_INT_BOUND :: 1000.
$ MAXIMUM_WAVENUMBER :: 1025.

$ WIDE_INTERVAL_SPAC :: 1.
$ WN_RANGE_FOR_FINE :: 1.
$ WN_RANGE_CONSIDER :: 25.
$ DIVISION_WIDE_FINE :: 500
$ NUM_PER_HALFWIDTH :: -1

!-------------------------------------------------------------------------------
* PTHFIL
-------------------------
$ USER_PROFILE : 'user profile' or 'model profile' are mandatory !
$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'
$ FLAG_ADD_ON
$ ADD_ON_FILE_NAME :: 'glatm.dat'
$ ADD_ON_PROF_NUMBER : tropical profile : 1

-------------
!$ MODEL_PROFILE : 'user profile' or 'model profile' are mandatory !
!$ MODPRO_FILE_NAME :: 'glatm.dat'
!$ PROFILE_NUMBER :: 6

-------------
!$ REFRACTION

-------------
!$ USER_LAYERS
!$ LAYER_BOUND : H or P: 'H'
!$ LAYER_NUMBER :: 24
!$ SUB_LAYER_NUMBER :: 10

!$ LAYER_TABLE :
  1  0.00  1.10
  2  1.10  2.16
  3  2.16  3.04
  4  3.04  3.92
  5  3.92  4.82
  6  4.82  5.74
  7  5.74  6.64
  8  6.64  7.52
  9  7.52  8.42
 10  8.42  9.34
 11  9.34 10.28
 12 10.28 11.24
 13 11.24 12.22
 14 12.22 16.72
 15 16.72 21.16
 16 21.16 25.94
 17 25.94 30.80
 18 30.80 35.12
 19 35.12 39.62
$ DEFAULT_LAYERS : 'mandatory or user layers'

$ SUB_LAYER_NUMBER :: 10

$ MAX_VAR_VOIGT_HW : (should be between 1 and 2) : 2.0
$ MAX_TEMP_DIFF_BOT : Kelvin : 5.0
$ MAX_TEMP_DIFF_TOA : Kelvin : 30.0

!-------------------------------------------------------------------------------
* MIXFIL

$ NUMBER_MIXPATHS : or mixpath filename: 24

!$ MIXPATH_FILE_NAME : or number_mixpaths: ''

$ MIXING_TABLE :
  1 R0T0 1 R0T23 R0T0 1 R0T23 R0T0 1 R0T23
  2 R0T1 1 R0T22 R0T1 1 R0T22 R0T1 1 R0T22
  3 R0T2 1 R0T21 R0T2 1 R0T21 R0T2 1 R0T21
  4 R0T3 1 R0T20 R0T3 1 R0T20 R0T3 1 R0T20
  5 R0T4 1 R0T19 R0T4 1 R0T19 R0T4 1 R0T19
  6 R0T5 1 R0T18 R0T5 1 R0T18 R0T5 1 R0T18
  7 R0T6 1 R0T17 R0T6 1 R0T17 R0T6 1 R0T17
  8 R0T7 1 R0T16 R0T7 1 R0T16 R0T7 1 R0T16
  9 R0T8 1 R0T15 R0T8 1 R0T15 R0T8 1 R0T15
 10 R0T9 1 R0T14 R0T9 1 R0T14 R0T9 1 R0T14
 11 R0T10 1 R0T13 R0T10 1 R0T13 R0T10 1 R0T13
 12 R0T11 1 R0T12 R0T11 1 R0T12 R0T11 1 R0T12
 13 R0T12 1 R0T11 R0T12 1 R0T11 R0T12 1 R0T11
 14 R0T13 1 R0T10 R0T13 1 R0T10 R0T13 1 R0T10
 15 R0T14 1 R0T9  R0T14 1 R0T9  R0T14 1 R0T9
 16 R0T15 1 R0T8  R0T15 1 R0T8  R0T15 1 R0T8
 17 R0T16 1 R0T7  R0T16 1 R0T7  R0T16 1 R0T7
 18 R0T17 1 R0T6  R0T17 1 R0T6  R0T17 1 R0T6
 19 R0T18 1 R0T5  R0T18 1 R0T5  R0T18 1 R0T5
 20 R0T19 1 R0T4  R0T19 1 R0T4  R0T19 1 R0T4
 21 R0T20 1 R0T3  R0T20 1 R0T3  R0T20 1 R0T3
 22 R0T21 1 R0T2  R0T21 1 R0T2  R0T21 1 R0T2
 23 R0T22 1 R0T1  R0T22 1 R0T1  R0T22 1 R0T1
 24 R0T23 1 R0T0  R0T23 1 R0T0  R0T23 1 R0T0

!-------------------------------------------------------------------------------

*RADNCE

$ NUMBER_OF_RADIATING_ATMOSPHERES :: 1

$ MAXIMUM_NUMBER_OF_LAYERS_PER_ATMOSPHERE :: 24

$ LAYER_TABLE
  1  2  1  24  1  24  23  22  21  20  19  18  17  16  15  14  13  12  11  10  9  8  7  6  5  4  3  2  1
  3.0  0.0  1.0000

!-------------------------------------------------------------------------------

* OUTPUT

$ OUTPUT_FILE_NAME :: 'ex1_genln3_op_zenith_calc_looking_upward.ncdf'
8.7.3 Example 7: Output

Figure 19: Example 7 (Radiance looking upward through atmosphere to space): Emission spectra between selected atmospheric levels and TOA. The atmosphere contains $H_2O$, $CO_2$, $O_3$, and $CFC12$. The bottom plot is the spectrum measured at the surface.

8.8 Example 8: NADIR calculation which includes sulfate aerosol

link_to_g3_tech_note_example_8_NADIR_WITH_AEROSOL
8.8.1 Example 8: HITRUN Input File

Same as Example 1.

8.8.2 Example 8: GENRUN Input File

* TITLES

TITLE : Overall title : 'ex1 NADIR HT2012 w/ aerosol'

* DEFGRD

MINIMUM_WAVENUMBER :: 825.
LOWER_INT_BOUND :: 850.
UPPER_INT_BOUND :: 1000.
MAXIMUM_WAVENUMBER :: 1025.
WIDE_INTERVAL_SPAC :: 1.
WN_RANGE_FOR_FINE :: 1.
WN_RANGE_CONSIDER :: 25.
DIVISION_WIDE_FINE :: 100.
NUM_PER_HALFWIDTH :: -1

* GEOMET

MODE :: 'NADIR'
ATM_BOUND : H or P : 'H'
ATM_LOWER_BOUND :: 0.
ATM_UPPER_BOUND :: 80.
VIEW_ZENITH :: 0.0
AZIMUTH :: 0.0
TEMP_UPPER_BOUND :: 2.96
TEMP_SURFACE :: 293.2
EMISSIVITY_SURFACE :: 0.9889
SUN_ZENITH :: 0.0

* OUTPUT

OUTPUT_FILE_NAME :: 'ex1_genln3_op_NADIR_with_aerosol.ncdf'

TRANSMITTANCE

OPTICAL_DEPTH

RADIANCE

RADIANCE_COMPONENTS

GAS_CONTRIBUTIONS

FINE

ALL_LAYERS

* GASFIL

LINE_MIXING
$ NUMBER_OF_FILES :: 1
$ LINE_CUTOFF_WIDE :: 0.0
$ LINE_CUTOFF_FINE :: 0.0

$ GAS_FILE_NAME
'hitlin_op_475_1700_HT2012_WITH_CO2_LINMIX.bin'
$ NUMBER_OF_GASES
4

$ GAS_TABLE
1, 0, 'VOIGT', 'CON' , 10
2, 0, 'VOIGTCO2', 'CON' , 11
3, 0, 'VOIGT', 'NOCON' , 10
91, 0, 'AEROSOL', 'NOCON' , 10

---------------------------------------------------------------------

* PTHFIL

$ USER_PROFILE : 'user profile' or 'model profile' are mandatory!

$ PROFILE_FILE_NAME :: 'ex1_layers_pro.dat'

$ FLAG_ADD_ON
$ ADD_ON_FILE_NAME :: 'glatm.dat'
$ ADD_ON_PROF_NUMBER :: 2

---------------

!* MODEL_PROFILE : 'user profile' or 'model profile' are mandatory!

!* MODPRO_FILE_NAME :: 'glatm.dat'
!* PROFILE_NUMBER :: 6

---------------

!* REFRACTION

---------------

$ USER_LAYERS

$ LAYER_BOUND : H or P: 'H'
$ LAYER_NUMBER :: 24
$ SUB_LAYER_NUMBER :: 10

$ LAYER_TABLE :
1  0.000  1.100
2  1.100  2.200
3  2.200  3.100
4  3.100  4.000
5  4.000  4.900
6  4.900  5.800
7  5.800  6.700
8  6.700  7.600
9  7.600  8.500
10 8.500  9.400
11 9.400 10.400
12 10.400 11.400
13 11.400 12.400
14 12.400 16.900
15 16.900 21.400
16 21.400 26.300
'DEFAULT LAYERS' : 'mandatory or user layers'

'SUB_LAYER_NUMBER' :: 10

'MAX_VAR_VUIGT_HW' : (should be between 1 and 2) : 2.0

'MAX_TEMP_DIFF_BOT' :(K) : 5.0

'MAX_TEMP_DIFF_TOA' :(K) : 30.0

* XSCFIL

$ PATH_TO_XSFILES : trailing '/' : 'HIT2012/IR-XSect/Uncompressed-files/'

$ NUMBER_OF_GASES :: 1

$ MOLECULE_IDS : -number of gases- values : 52

* MIXFIL

$ NUMBER_MIXPATHS : or mixpath filename: 28

$ MIXPATH_FILE_NAME : or number mixpaths: ''

$ MIXING_TABLE :

1  ROT0 1  ROT23  ROT0 1  ROT23  ROT0 1  ROT23
2  ROT1 1  ROT22  ROT1 1  ROT22  ROT1 1  ROT22
3  ROT2 1  ROT21  ROT2 1  ROT21  ROT2 1  ROT21
4  ROT3 1  ROT20  ROT3 1  ROT20  ROT3 1  ROT20
5  ROT4 1  ROT19  ROT4 1  ROT19  ROT4 1  ROT19
6  ROT5 1  ROT18  ROT5 1  ROT18  ROT5 1  ROT18
7  ROT6 1  ROT17  ROT6 1  ROT17  ROT6 1  ROT17
8  ROT7 1  ROT16  ROT7 1  ROT16  ROT7 1  ROT16
9  ROT8 1  ROT15  ROT8 1  ROT15  ROT8 1  ROT15
10  ROT9 1  ROT14  ROT9 1  ROT14  ROT9 1  ROT14
11  ROT10 1  ROT13  ROT10 1  ROT13  ROT10 1  ROT13
12  ROT11 1  ROT12  ROT11 1  ROT12  ROT11 1  ROT12
13  ROT12 1  ROT11  ROT12 1  ROT11  ROT12 1  ROT11
14  ROT13 1  ROT10  ROT13 1  ROT10  ROT13 1  ROT10
15  ROT14 1  ROT9  ROT14 1  ROT9  ROT14 1  ROT9
16  ROT15 1  ROT8  ROT15 1  ROT8  ROT15 1  ROT8
17  ROT16 1  ROT7  ROT16 1  ROT7  ROT16 1  ROT7
18  ROT17 1  ROT6  ROT17 1  ROT6  ROT17 1  ROT6
19  ROT18 1  ROT5  ROT18 1  ROT5  ROT18 1  ROT5
20  ROT19 1  ROT4  ROT19 1  ROT4  ROT19 1  ROT4
21  ROT20 1  ROT3  ROT20 1  ROT3  ROT20 1  ROT3
22  ROT21 1  ROT2  ROT21 1  ROT2  ROT21 1  ROT2
23  ROT22 1  ROT1  ROT22 1  ROT1  ROT22 1  ROT1
24  ROT23 1  ROT0  ROT23 1  ROT0  ROT23 1  ROT0
25  ROT24  ROT24  ROT24
26  ROT24  ROT24
27  ROT24  ROT24
28  ROT24  ROT24
! AEROSOL DATA
! EXAMPLE USING H2SO4 AEROSOL
! keyword
! aerosol file name(s)
! number of gasids
! gasid(s)
! normalization wavenumber

* AERFIL

$ AEROSOL_FILE_NAME :: 'aero.dat'
$ NUMBER_AEROSOLS :: 1
$ AEROSOL_IDS :: 91
$ NORMALIZATION_WN :: 1250.

* ENDINP
8.8.3 Example 8: Output

Figure 20: Example 8 (NADIR calculation incorporating sulfate aerosol): Individual transmittance spectra for $H_2O$, $CO_2$, $O_3$, $H_2SO_4$, and $CFC12$. Also the total transmittance of all gases calculated two ways, and their (small) difference.
References


Birch, K. P., and M. J. Downs, Correction to the updated Edlén equation for the refractive index of air, Metrologia 31, 315-316 (1994).


Burch, D. E., and R. L. Alt, Continuum Absorption by $H_2O$ in the 700-1200 cm$^{-1}$ and 2400-2800 cm$^{-1}$ windows, AFGL-TR-84-0128, AFGL (OPI), Hanscom AFB, MA 01731, 1984.


