

User's Guide for UNL–VRTM

A UNified Linearized Vector Radiative Transfer Model

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Recent UNL-VRTM Versions

Version	Date	git ID	Remark
1.4.6	24 Nov 2015	dd3d48a	User atmos profile; Loc/time SZA; Gas lookup table
1.4.5	28 Oct 2015	fd97a10	netCDF update; Frequency input; Aerosol profile bugfix
1.4.4	27 Sep 2015	a167d48	Cloud treatment verified
1.4.3	15 Sep 2015	632bc68	Surface-leaving verified
1.4.2	01 Jul 2014	464e7ea	More surface types; Surface-leaving
1.4.0	01 Jul 2014	79831f1	First-time git; AERONET inversion
1.3.0	Early 2014	n/a	Public released version

Recent Updates

New in v1.4.6

- User-specified atmospheric profile is now enabled. The model could read height and pressure grid, air temperature and gasesou profiles from a well-prepared text file (atmos.dat) or a netCDF file (atmos.nc). Aerosol vertical profiles may also be read from the same file.
- Option has been added to calculate the solar position given the observing location and time.
- Gas cross-section lookup table facility. This facility will benefit the hyperspectral calculations which usually involved a great number of spectra over a wide spectral range. With this facility, model only does the LBL calculation once for given spectral samplings and save the gas cross-section data for each atmospheric layer, and the subsequent running will read these data and calculate the cross-section from the same (or interpolated from the neighboring) pressure level. A calculation in full IR (500–2500 cm^{-1} originally takes about 50 min. Now it is reduced to 40 sec with the lookup table.

New in v1.4.5

- The netCDF utility is fully rewritten. Now we have (1) all diagnostic fields saved in a single netCDF file, (2) improved the self-descriptive capability of the output by adding many global attributes, and (3) option of netCDF3/netCDF4 formats.
- Bug fixing for exponential-decreasing aerosol vertical profile.
- Enabled the option for spectral frequency inputs.

1 Getting Start

1.1 Obtaining the UNL-VRTM

Model packages including source code and run directories are available through the Git repository on <https://gitlab.com>. This Quick Start Guide goes through the process of how to create an account get the latest version of the code.

To access to the code, you will need to create an account on <https://gitlab.com> and tell me your username on this account. I will add you as a member of the UNL-VRTM project so that you could view, download, and even make comments/contributions on the project. Once you have familiarized yourself with the Git environment you may proceed. More information on Git is at [Git Documentation](#) and [Git Man Page](#). Please review this online documentation for a better understanding of using Git.

Initial download After you joined the UNL-VRTM project on <https://gitlab.com>. You can download the most current copy of the code by entering the following command on you local Linux terminal:

```
git clone git@gitlab.com:xxu/unlvrtm.git
```

This will download a project directory *unlvrtm* containing the source code and run directories.

Tracking subsequent changes by yourself and others Perhaps you already have a version of model. To determine the status of your existing project vs the current repository version, enter your local copy of your project directory and type

```
git status
```

To further determine the difference between your local copy and the current repository copy, type

```
git diff --word-diff=color origin/master
```

The `word-diff=color` option makes the output with colors so it is easy to read, specifying `origin/master` takes the difference between your copy and the newest repository copy. Without `origin/master`, you will see the difference between your copy and the version that was in the repository as of the last time you checked out the code. The commands above are without arguments and will thus apply to all files in the project. To use them for only one specific file, for example `main.f`, type:

```
git diff --word-diff=color origin/master --main.f
```

To replace your local copy of `main.f` with the newest version from the repository,

```
git checkout origin/master -- main.f
```

If you have also modified your local copy, you can merge your changes with those made to the repository version

```
git checkout --patch origin/master -- main.f
```

If you want your updates to be added to the main repository please create a PATCH and contact the Development Team. Richard will handle incorporating changes into the code repository. Please do not distribute copies of the code at this time; you may refer such requests to the authors.

1.2 Directory Structure Overview

The package consists of several subdirectories. If you are in the root directory, a *ls* command should give you:

```
doc/  run/  src/  util/
```

A short description of each subdirectory is as following:

- The *doc* contains relevant documents, such as the user's guide and instructions.
- The *src* is the subdirectory for the source code. It also includes the Fortran libraries of linearized Mie/T-Matrix code and VLIDORT (version of 2.6) model.
- The *run* is used to run the model, which contains the necessary namelist file and input files.
- The *util* folder consists some analysis tools for the model outputs, including IDL routines.

In addition, the model needs input of a set of ancillary data, including the gaseous spectroscopic line parameters and cross section database, which are stored in a *data* folder. Users needs to obtain those data from the model developer, and specify the path for *data* in the model input file.

1.3 Compile UNL-VRTM

A full compilation is necessary when you first get the codes. It could be done by executing the file *compile* in the *src* folder, which will compile UNL-VRTMall and all of the necessary libraries.

Later if you made revisions about the codes but not the libraries, you could compile UNL-VRTM with the Makefile stored in in the *src* folder. Type ‘make clean’ to clear the compiled modules, and type ‘make -f Makefile’ to perform a new compilation.

It should be noted that, we have compiled the model only with Intel fortran compiler (ifort). Error may be encountered if other compilers are used.

1.4 Run UNL-VRTM

To run the model, just move/copy the generated executable file *unlvrtm.exe* upon compilation to the *run* directory, and run it with the specification of the input file *namelist.ini*. A detail description on how to set the model input in section 2.

Running the UNL-VRTM requires large amount of memory and large stack size. We recommend run the model through submitting a job with the scheduler on Linux system. Users can adopt the run script *run.sh* to the specific scheduler and use it to run the model. If you like to execute the model directly, make sure to type below lines before running to set an unlimited memory and enlarge the stake size:

```
ulimit -s unlimited
export KMP_STACKSIZE=209715200
```

Above two lines are bash commands. You will need to apply corresponding syntax if you use a differenty type of shell (like csh) on your machine.

2 Input Files

This chapter describes the necessary and optional input files of the model. One mandatory input file is *namelist.ini* located in the *run* directory. It is used to specify the modeling settings for desired simulation. Depending on the specified settings, optional input files may be needed. These include a file named *spectra.dat* defining the spectral samplings and a file providing atmospheric profiles.

2.1 Mandatory input file: *namelist.ini*

We put all the run options and switches into this single input file. It should be placed in the run directory. In this file, users may specify most of the options for the radiative transfer simulation, including spectral samplings, atmospheric profiles, air molecular optics, aerosol physical and optical properties, surface property, and diagnostics to be saved, etc. Note that these model settings are grouped into menus in *namelist.ini*, as following the style and logic from the input file of GEOS-Chem model (www.geos-chem.org). Each menu controls the options for a particular aspect of the model. Below is a list of the menus and the options which they control.

- **Control Menu** specifies the spectral information, atmosphere type, and directory information.
- **Geometry Menu** specifies the sun-earth-viewer geometry.
- **RTM Menu** specifies the simulation options for the VLIDORT model.
- **Jacobian Menu** specifies the parameters to be included for Jacobian calculations.
- **Surface Menu** specifies the surface optical properties.
- **Aerosol Menu** specifies the optical and physical properties of aerosol.
- **Tracegas Menu** specifies the information of each trace gas, including name, molecular weight, and the individual switch.
- **Rayleigh Menu** specifies the Rayleigh scattering calculation.
- **Diagnostic Menu** specifies which variables are saved to output.

- **Debug Menu** includes switches of debugging some aspect of the model.

Each of these menus is described in more detail below. Note that the line numbers are not part of the file *namelist.ini*, but have been included for the convenience of interpretation.

2.1.1 The CONTROL Menu

```

1  %%% CONTROL MENU %%%      :
2  Frequency as input?      : F
3  Spectra set (nm or 1/cm): 755 775
4   - interval(nm or 1/cm): 1
5   - FWHM    (nm or 1/cm): 2
6  Atmos. type[1-6,-1,or-2]: 2
7  # of atmos. layers      : -1
8  Run   directory        : ./
9  Data  directory        : /work/jwang7/xxu/ARTDATA/data/
10 Output directory       : ./results/

```

Description:

1. Title for this menu.
2. Switch to turn on/off the frequency as spectral input for the following three lines: A "T" is for frequency-mode input in the units of cm^{-1} ; An 'F' is for wavelength input in the units of nanometer (nm).
3. Specifies the spectral range in the units of nanometer or cm^{-1} . User can specify either a single spectrum or multiple spectra. It should be noted that, for multiple spectrum, the input values should be in an ascending sequence.
4. Specifies the sampling step for the spectrum in nm or cm^{-1} .
5. Specifies the spectral resolution for each spectral sampling in terms of the full-width at half maximum (FWHM) for an assumed Gaussian-shape spectral response.

Please note that there are various options for specifying spectrum with above line 3 and line 4:

- If only one wavelength is specified in line 3, or value of zero is in line 4, the model will perform the simulation on a single wavelength.
 - If two wavelengths are specified in line 3, and an interval specified in line 4, model will simulate multi-spectrum from starting spectrum to the ending spectrum with the equal intervals. For example, With above spectral settings the model will do simulation in the O2-A band (755–775 nm) with equal interval of 1 nm at the spectral resolution (FWHM) of 2 nm.
 - If three or more spectral values are specified in line 3, the simulation will be performed exactly on these specified spectra. The specified spectral interval value does not take effects.
 - If an "-1" is put in line 3, model will read spectral settings from a file named *spectra.dat* (see Section 2.2).
6. Specifies the index of atmospheric type for the meteorological and air density profile. Number of 1 to 6, or -1 indicate 6 different atmospheric profile types (adopted from *Optical Properties Of The Atmosphere*, Third Edition, AFCRL-72-0497; *U.S. Standard Atmosphere 1976*) or user specified profiles.
- 1: Tropical
 - 2: Mid-latitude summer
 - 3: Mid-latitude winter
 - 4: High-latitude summer
 - 5: High-latitude winter
 - 6: US standard (1976)
 - -1: User specified in an *atmos.dat* file (in developing)
 - -2: User specified in an *atmos.nc* file
7. Specifies the number of atmospheric layers. Those built-in atmospheric types are 49 layers and options for this number are:
- 49: Full standard atmospheric profile with 49 layers.
 - Any number from 1 to 48: Uses the specified number of bottom layers.
 - -1: 33 atmospheric layers, by aggregating a few stratospheric layers.
 - -2: 26 atmospheric layers, by aggregating a more stratospheric layers.

- -3: 3 atmospheric layers, with 2 layers in troposphere and 1 in stratosphere.

If user-specified atmospheric profile is used, the layer number specified here must be same to the number of layer stored in the user-specified data file.

8. Specifies the model run directory. Generally, it is `"/` which indicates the current directory.
9. Specifies the directory where the ancillary data is placed.
10. Specifies the subdirectory where the model output will be saved.

2.1.2 The GEOMETRY Menu

```

1  %% GEOMETRY MENU %%   :
2  Solar zenith angle    : 30
3  Solar azimuthal angle : 0
4  Solar position by time? : F
5   - yyyyymmdd hhmss    : 20120101 103000
6   - latitude longitude : 10 -20
7  Viewer zenith angles  : 0
8  Relative azimuth angles : 0

```

Description:

1. Title of geometry menu
2. Specifies solar zenith angle. You may list a single or multi angles in the units of degree. However, from version 1.4.6 you could put only a single solar zenith angle.
3. Specifies azimuthal angle in degree.
4. Switch to turn on/off the calculation of solar zenith and azimuthal angles from below specified latitude/longitude and date/time. And the solar angles from above two lines will be replaced.
5. Specifies the date/time in an integer format of YYYYMMDD and hhmss.
6. Specifies the latitude and longitude of the observing location in degree.

7. Specifies viewing zenith angles. You may list one or more (up to 4) values.
8. Specifies the relative azimuth angles, number of which is also up to 2.

However, it should be noted that user can increase, if needed, those maximum numbers for each type of angles by modifying a VLIDORT code and updating the library of VLIDORT. This will be discussed in Chapter 4.

2.1.3 The VLIDORT Menu

```

1  %% RTM MENU %%           :
2  Turn on RTM (VLIDORT)?   : T
3  # of Stokes components   : 3
4  # of discrete streams    : 15
5  # of P Legendre terms    : 100
6  Receptor levels          : 0
7  Receptor direction       : -1
8  Do pseudo-spherical?    : T
9  SS correction scenario   : 1
10 Do solar source          : F
11  - flux factor           : 1.0
12 Do atmos emission?      : T
13 Do surface emission?    : T
14  - surface T (K)        : 300.

```

Description:

1. Title for VLIDORT menu.
2. Switch to turn on/off the VLIDORT calculation
3. Specifies the number of Stokes vector components $[I, Q, U, V]$. By setting 1, the model will be only calculating I . By setting 3, model calculates I, Q, U , and similarly, model calculates full Stokes vector if 4 is set.
4. Specifies number of streams in the hemisphere.
5. Specifies number of Legendre expansion terms for Greek Matrix. Current maximum is 180, but user can increase it (see Chapter 4).
6. Defines on which levels you want to calculate the radiance. The maximum number of levels is 2. Note that level is 0 to N from the top-of-atmosphere

(TOA) to the bottom-of-atmosphere (BOA) in VLIDORT. Therefore, **0 represents TOA level**. For the convenience, you may also use -1 to indicate the BOA level.

7. Specifies the direction of beam to the viewer. **-1 and 1 represent upward and downward**, respectively.
8. Switch to turn on/off the pseudo-spherical approximation of the atmosphere through the light-of-path. A plane-parallel atmosphere is considered if it is off.
9. Specifies the scenario of the single scattering correction in VLIDORT. Please check the code *vlidort_mod.f* for detail. 0 is recommend for Rayleigh only atmosphere; while 1 is recommended if aerosol scattering involves. 2 or 3 can should be used if an optically thick layer (like cloud) presents.
10. Switch to turn on/off the solar radiant source.
11. Specifies the solar irradiance factor, default value is one.
12. Switch to turn on/off atmospheric thermal emissions.
13. Switch to turn on/off surface thermal emission (atmospheric thermal emission must be on in order to turn this on).
14. Specifies the surface temperature for the surface thermal emission.

2.1.4 The JACOBIAN Menu

```
1  %%% JACOBIAN MENU %%%   :
2  Turn on atmos. Jacob.?  : T
3   - wrt Gas?             : F
4   - wrt AOD?             : F
5   - wrt SSA?             : F
6   - wrt aerosol volume?  : T
7   - wrt mode fraction?   : F
8   - wrt refractivity?    : T
9   - wrt shape factor?    : F
10  - wrt size dist?       : T
11  - wrt vertic profile?  : F
12  Non-varying volume?    : T
13  Non-varying AOD?      : F
14  Turn on surface Jacob.? : T
```

```
15 - wrt BRDF factor?      : T
16 - wrt BRDF parameter?  : F
17 Do FD verification?    : F
```

Description:

1. Title for Jacobian menu.
2. Switch to turn on/off the calculation for Jacobian for atmospheric trace gas or aerosol parameters. If set false, all the atmospheric Jacobian calculations will be turned off.
3. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to total gas absorption optical depth.
4. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol optical depth.
5. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol single scattering albedo.
6. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol volume.
7. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol modal fraction.
8. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol refractive indices.
9. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol shape factor (with T-Matrix code turned on).
10. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol size distribution parameters.
11. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol vertical profile parameters.
12. If true, keep the mass constant (but varying AOD) in the Jacobian calculation.
13. If true, keep AOD as a constant (but varying mass) in the Jacobian calculation. Only one and must one of this and above one should be true.

14. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to surface reflectance.
15. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to BRDF amplitude factor of each kernel.
16. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to BRDF kernel parameters.
17. Switch to turn on/off the finite difference verification for the Jacobian calculation of VLIDORT model (current not useful, may be removed later!).

2.1.5 The SURFACE Menu

```

1 %%% SURFACE MENU %%%      :
2 Do Lambertian surface?   : F
3   - surface reflecetance: 0.1
4 Do BRDF surface?        : T
5   - # of BRDF kernels    : 3
6   - BRDF kernel entries : Name      Index  Factor  #PARS  PAR(1)  PAR(2)  PAR(3)
7       ==> kernel#1 : Lambertian  1     0.18   0     0.0    0.0    0.0
8       ==> kernel#2 : Ross-thick  3     0.10   0     0.0    0.0    0.0
9       ==> kernel#3 : Li-sparse   4     0.03   2     2.0    1.0    0.0

```

Description:

1. Title for the Surface Menu.
2. Switch to turn on/off the Lambertian surface.
3. Define the Lambertian surface reflectance value. A decimal value between 0 and 1 (include 0 and 1) indicates a specified surface reflectance value. An integer of -1 will let the model get the surface reflectance from the *spectra.dat* file (an integer of -1 is also required for line 3 in the CONTROL menu, section 2.1.1). Alternatively, by setting a integer number from 2 to 8, the model will use its built-in reflectance spectrum library:
 - 2: tap-water surface
 - 3: sea-water surface
 - 4: fine-snow surface

Table 2.1: Summary of available BRDF kernels (from VLIDORT User’s Guide).

Index	Kernel Name	# Pars	Type	Source
1	Lambertian	0	Scalar	
2	Ross-thick	0	Scalar	Wanner et al., 1995
3	Ross-thin	0	Scalar	MODIS
4	Li-sparse	2	Scalar	MODIS
5	Li-dense	2	Scalar	MODIS
6	Roujean	0	Scalar	MODIS
7	Rahman(RPV)	3	Scalar	Rahman et al., 1993
8	Hapke	3	Scalar	Hapke, 1993
9	Cox-Munk	2	Scalar	Cox/Munk, 1954
10	GISS Cox-Munk	2	Vector	Mishchenko/Travis 1997
11	BPDF2009	2	Vector	Maignan et al., 2009

- 5: medium-snow surface
- 6: surface with deciduous trees
- 7: surface with green grasses
- 8: surface with gry grasses

4. Switch to turn on/off the BRDF surface. It should be noted that only and must one of Lambertian and BRDF should be set true.
5. Define number of used BRDF kernels (maximum is 3).
6. BRDF entry titles.
7. From line 7 are the parameters for each kernel:(1) Kernel names, (2) kernel index, (3) amplitude of the kernel, (4) number of parameters, (5) kernel parameters up to 3. (Table 2.1 lists the available kernels, but more details are referred to VLIDORT User’s Guide).

2.1.6 The AEROSOL Menu

```

1 %%% AEROSOL MENU %%%      :
2 Turn on aerosol?          : T
3 Number of aerosol modes   : 2
4 Modal fractions           : 0.65      0.35
5 Columnar AOD as input?    : F         1.0

```



```

6 Columnar Vol as input? : T          0.20
7 Mie(1) or T-Matrix(2)? : 1          1
8 Mode #1 Properties     : .....Mode#1.....
9   - refractive index   : 1.33E+00  0.006
10  - shape factor        : -1         1.4
11  - monodisperse?      : F         1.0
12  - size range [um]    : 0.01       15
13  - size distribution   : Index    PAR(1)   PAR(2)   PAR(3)
14      ==> Entries : 4          0.1     1.6     0
15  - vertical range[km] : 0         15
16  - vertical profile   : Index    PAR(1)   PAR(2)
17      ==> Entries : 3          0.5     2.0
18 Mode #2 Properties     : .....Mode#2.....
19  - refractive index   : 1.53E+00  0.001
20  - shape factor        : -1         1.0
21  - monodisperse?      : F         1.0
22  - size range [um]    : 0.05      15.0
23  - size distribution   : Index    PAR(1)   PAR(2)   PAR(3)
24      ==> Entries : 4          1.00    2.0     0
25  - vertical range[km] : 0         15.0
26  - vertical profile   : Index    PAR(1)   PAR(2)
27      ==> Entries : 3          2.0     2.0
28 Reference aerosol mode : .....Mode#REF.....
29  - reference AOD?      : F
30  - wavelength [nm]    : 354
31  - refractive index   : 1.75E+00  0.435
32  - monodisperse?      : F         1.0
33  - size range [um]    : 0.01      10.0
34  - size distribution   : Index    PAR(1)   PAR(2)   PAR(3)
35      ==> Entries : 4          0.01    2.0     0

```

Description:

1. Title for aerosol menu.
2. Set true to include aerosol scattering for the radiance calculation.
3. Specifies number of aerosol modes. 1 for single mode, 2 for bi-mode.
4. Specifies the modal fractions. If single mode, this line is non-effective. Note that these could be either AOD fractions or mass fractions, depending on which is used as loading input in following two lines.
5. Define the column atmospheric aerosol optical depth (AOD). (1) Turn on/off using column AOD as aerosol loading inputs; (2) Column AOD.

6. Define the column aerosol mass in the units of [kg/m²]. (1) Turn on/off using columnar volume as aerosol loading inputs. (2) Aerosol columnar volume in the units of $\mu\text{m}^3\mu\text{m}^{-2}$. NOTE that only one of volume and AOD as input should be turned on.
7. Specifies the used approaches for aerosol optical property calculation, **1 for Mie theory**, and **2 for T-Matrix method**. Two inputs are respectively for each individual modes.
8. Title for mode #1.
9. Refractive index for mode #1, respectively, real and imaginary terms. It should be noted that these refractive index is replaced by the values read from file *spectra.dat* if spectral range is specified as "-1" (line 3 in the CONTROL menu, section 2.1.1).
10. Shape factor for non-spherical particle when using T-Matrix calculation [details to be filled.....]
11. Options for mono-disperse simulation: (1) Turn on/off considering mono-disperse, (2) specify the mono-size in micron-meter.
12. Particle size range in micron-meter.
13. Size distribution entries titles
14. Size distribution entries: (1) Size distribution function index, (2)-(4) size distribution parameters, up to 3 parameters. Size distribution functions and their parameters are listed in Table 2.2.
15. Vertical extending range in [km].
16. Vertical profile entry titles.
17. Vertical profile function index, and parameters. See Table 2.3. Equations for index #2: $\int_{TOA}^z \tau(z)dz = \tau_0 \exp(-\frac{z}{H})$, where τ_0 is columnar AOD. The profile #3 follows an "almost-Gaussian" function: $\tau(z) = K \frac{\exp(-\sigma|z-z_{peak}|)}{[1+\exp(-\sigma|z-z_{peak}|)]^2}$, where K is related to the columnar loading, z_{peak} is the height of AOD peak, and σ related to the width.

Table 2.2: Summary of particle size distribution (PSD) options.

Index	Description of PSD and parameters
1	Two parameter GAMMA with ALPHA and B given
2	Two parameter GAMMA with REFF and VEFF given
3	3-parameter Bimodal equal-weight GAMMAS with 2 REFFs + same VEFF
4	Two parameter Lognormal with RG and SIGMA given
5	Two parameter Lognormal with REFF and VEFF given
6	Power-Law with R1, R2 and ALPHA
7	3-parameter Modified-Gamma with ALPHA,GC,GAMMA given
8	3-parameter Modified-Gamma with ALPHA,B,GAMMA given

Table 2.3: Summary of aerosol vertical profile options.

Index	Description of PSD and parameters
1	Uniform profile—aerosol are evenly distributed in the given vertical range
2	Exponentially decreasing profile with scale height H given
3	Generalized Distribution function, given z_{peak} and σ

18. Line 18 – 27: Specifies aerosol parameters for mode #2, similar to that of mode #1.
19. Line 28 – 35: Specifies aerosol parameters for a reference aerosol AOD value, similar to that of mode #1. The reference AOD can be used here when one knows the AOD values at certain wavelength and want to conduct simulation on other spectral wavelengths.

2.1.7 The TRACEGAS Menu

```

1  %%% TRACE-GAS MENU %%%  :
2  Turn on trace gases?    : T
3  Use pre-calculated data?: T
4  - give the data file   : clarreo.unlvrtm.nc
5  Num. of trace gases    : 22
6  Trace gas Entries      ==> : TR#   Name     M-Weight  Include?  Scaling
7  Trace gas #1           :    1   H2O      18.015    T         0.15
8  Trace gas #2           :    2   CO2     44.010    T         1.0
9  Trace gas #3           :    3   O3      47.998    T         1.25
10 Trace gas #4           :    4   N2O     44.010    T         1.0
11 Trace gas #5           :    5   CO      28.011    T         1.0

```

12	Trace gas #6	:	6	CH4	16.043	T	1.0
13	Trace gas #7	:	7	O2	31.999	T	1.0
14	Trace gas #8	:	8	NO	30.010	T	1.0
15	Trace gas #9	:	9	SO2	64.060	T	1.8
16	Trace gas #10	:	10	NO2	46.010	T	1.8
17	Trace gas #11	:	11	NH3	17.030	F	1.0
18	Trace gas #12	:	12	HNO3	63.010	F	1.0
19	Trace gas #13	:	13	OH	17.000	T	1.0
20	Trace gas #14	:	14	HF	20.010	F	1.0
21	Trace gas #15	:	15	HCL	36.460	F	1.0
22	Trace gas #16	:	16	HBR	80.920	F	1.0
23	Trace gas #17	:	17	HI	127.91	F	1.0
24	Trace gas #18	:	18	CLO	51.450	F	1.0
25	Trace gas #19	:	19	OCS	60.080	F	1.0
26	Trace gas #20	:	20	H2CO	30.030	T	1.0
27	Trace gas #21	:	21	HOCL	52.460	F	1.0
28	Trace gas #22	:	22	N2	28.014	F	1.0

Description:

1. Title for trace gas menu.
2. Set true to include trace gas absorption for the radiance calculation.
3. Switch to turn on/off the option for using the pre-cauclated gas absorption cross-sections as a lookup table. See section 2.4 for a detail description of this option.
4. Specifies the netCDF file that contains pre-cauclated gas cross-sections.
5. Specifies the total number of considered trace gas. This **must** be 22 in the current version of the model.
6. Entries.
7. Line 7-28 give the tracer number, name, mole weight, switches to turn on/off the inclusion of each gas, and the scaling factor. The scaling factor scale the gaseous columnar amount from the built-in standard atmospheric profile. The value of 1.0 indicating to use the standard profile. And in practical, it is recommend to exclude gases those having zero or negligible absorption in your focused bands, which will considerably speed up the model run.

2.1.8 The RAYLEIGH Menu

```
1 %%% RAYLEIGH MENU %%% :  
2 Turn on Rayleigh?      : T  
3 Turn on anisotropy?    : T
```

Description:

1. Title for Rayleigh menu.
2. Set true to include atmospheric Rayleigh scattering for the radiance calculation.
3. Switch to turn on/off the anisotropy effect of atmospheric molecules.

2.1.9 The DIAGNOSTIC Menu

```
1 %%% DIAGNOSTIC MENU %%% :  
2 Turn on DIAGNOSTIC?     : T  
3 Output NC file prefix   : cntl  
4 DIAG01: Model inputs    : T  
5 DIAG02: Atmos profiles  : T  
6 DIAG03: Linearized Mie  : T  
7 DIAG04: Optic profiles  : T  
8 DIAG05: Surface property: T  
9 DIAG06: VLIDORT IOP     : T  
10 DIAG07: Radiances      : T  
11 DIAG08: Jacobians      : T
```

Description:

1. Title for diagnostic menu.
2. Switch to turn on/off of generating the diagnostic file.
3. Specifies a prefix name for the diagnostic file (netCDF format).
4. Switch to turn on/off of including the model input variables to the diagnostic file. Following lines are similar. A full list of output variables for each DIAG are presented in Chapter 3

2.1.10 The DEBUG Menu

```
1 %%% DEBUG MENU %%%      :
2 Write VLIDORT inputs?   : F
3 Turn on screen print?   : T
4 - print aerosol calc?   : F
5 - print Mie calc?       : F
6 - print Rayleigh calc?: F
7 - print gas calc?       : F
8 - print surface calc?   : F
9 - print RTM calc?       : F
```

Description: Debug menu includes switches to turn on/off screen debug output the calculation. These lines are straightforward and will not be explained in detail here.

2.2 Optional spectral input file: *spectra.dat*

The *spectra.dat* is an optional input file specifically designed for multi-spectrum simulations. If wavelengths option in Control Menu of *namelist.ini* (Section 2.1.1) is specified as below, the model will read wavelengths, aerosol refractive indices, and surface reflectance (Lambertian or BRDF) parameters from *spectra.dat*.

```
Spectra set (nm or 1/cm): -1
```

We recommend users use this optional input for multi-spectrum simulations when:

- Aerosol refractive indices varies on the interested wavelengths.
- Surface reflectance varies on the interested wavelengths.

By reading data from *spectra.dat*, the model will correspondingly perform the following configurations:

- The first column in *spectra.dat* is either spectral wavelength (nm) or spectral frequency (cm^{-1}) depending on if turning on/off the "Frequency as input". And the specified spectral FWHM still apply.
- Aerosol refractive index specified in the *namelist.ini* will be replaced by the refractive index from *spectra.dat* for each spectrum.

- If BRDF surface is considered, the BRDF amplification foactors for each kernel specified in the *namelist.ini* will also be replaced.
- If Lambertian surface is considered, a "-1" must specified for the surface reflectance value (as below) in order to have model use the surface reflectance specified in the *spectra.dat* file (the 6th column). Otherwise, surface reflectance will be defined as normal (Section 2.1.5).

```

Do Lambertian surface? : T
- surface reflecetance: -1

```

Here is an example of the file *spectra.dat* for an AERONET sky radiance simulation with four spectral wavelengths:

```

#1=====
#2 $id:spectra.dat, specifically for multi-spectral simulations by UNL-VRM
#3 - first 10 lines are used for comments
#4 - 11th line: specify number of spectrum
#5 - following lines wavelength(nm), n_real, n_img, n_real, n_img,
#6     - column#1 : wavelength(nm) or frequency (cm^-1) in ascending
#7     - column#2-5: n_real, n_img for 1st mode, and n_real, n_img for 2nd
#8     - column#6-8: amplification foactor for BRDF model
#9 Version 1.2.0, 4/29/2013, update v1.3, 8/26/13
#10=====
  4
440   1.478  0.0101   1.478  0.0101   0.0739  0.0357  0.0100
675   1.492  0.0071   1.492  0.0071   0.1392  0.0768  0.0202
870   1.493  0.0075   1.493  0.0075   0.1677  0.0894  0.0121
1020  1.488  0.0091   1.488  0.0091   0.1832  0.0764  0.0113

```

2.3 User-specified atmospheric profile: *atmos.dat/atmos.nc*

To give the model an user-specified atmospheric profile, you will need to specify "Atmos. type[1-6,-1,or-2]:" as "-1" or "-2" in *namelist.ini* and prepare a file that contains atmospheric profiling variables. In addition, the number of atmospheric layers specified in *namelist.ini* must be equal to the number of layers for the prepared profile. The file for profile will be *atmos.dat* in ASCII format for "-1" and *atmos.nc* in netCDF format for "-2". While we have implemented the option for reading data from *atmos.nc*, the *atmos.dat* option is still in developing. Below we describe how to prepare the netCDF file.

Table 2.4: List of variables in *atmos.nc*.

Variable	Type	Dimension	Units	MustHave	Description
ZGrid	real*4	(0:nLayer)	km	yes	Height grid (ascending) of layer edges
PGrid	real*4	(0:nLayer)	hPa	yes	Pressure grid of layer edges
T	real*4	(1:nLayer)	K	yes	Temperature of layers
H2O	real*4	(1:nLayer)	ppm	no	Water vapor mixing ratio
CO2	real*4	(1:nLayer)	ppm	no	Water vapor mixing ratio
...	no	Any given gas name
NYMD	integer	0	none	no	date in YYYYMMDD
NHMS	integer	0	none	no	time in hhmmss
Lon	real*4	0	degree	no	Longitude
Lat	real*4	0	degree	no	Latitude

The *atmos.nc* should contain a few must-have variables and several optional variables as listed in Table 2.4. By reading this file, the model will apply following configurations:

- The user-specified ZGrid, PGrid, and T will be used. Air molecular density at each layer will be derived from these quantities.
- If a given gas (with positive mixing ratio) is present in the file, the model will use specified gas profile. Otherwise, model will use the gas profile from a Standard Atmosphere.
- If model calculates solar position based on given time/location (see Section 2.1.2) and variables of NYMD, NHMS, Lon, and Lat are present in *atmos.nc*, model will read these variables and replace the time/location specified in the *namelist.ini* file.
- Future development may include aerosol profile in this file as well.

2.4 Pre-calculated gaseous LBL cross-section

Starting from version 1.4.6, we implemented gas cross-section lookup table facility. This facility will benefit the hyperspectral calculations which usually involved a great number of spectra over a wide spectral range. This is the case for simulating observation of a spectrometer with its prescribed spectral sampling and resolution.

With this facility, model performs the line-by-line (LBL) calculation only once for given spectral samplings and save the gas cross-section data for each atmospheric layer. The subsequent running will read these data and calculate the cross-section

from the same (or interpolated from the neighboring) pressure level. A calculation in full IR (500–2500 cm^{-1} originally takes about 50 min. Now it is reduced to 40 sec with the lookup table.

The procedure to use pre-calculated LBL is:

- Perform an online LBL calculation. This will be a regular simulation with trace gas turning on and the use of pre-calculated gas data off in the *namelist.ini* file:

```
Turn on trace gases?      : T
Use pre-calculated data?: F
.....
Turn on DIAGNOSTIC?      : T
Output NC file prefix    : lbl-lookuptable
.....
DIAG04: Optic profiles   : T
```

This simulation will yield a diagnostic file (*lbl-lookuptable.unlvrtm.nc*) according to above settings.

- Then perform subsequent simulations for same spectral definition use the pre-calculated gaseous cross-section data in *lbl-lookuptable.unlvrtm.nc*. To do so, just simply place this file in a safe place and modify the input file into:

```
Turn on trace gases?      : T
Use pre-calculated data?: T
- data filename           : the-foler/lbl-lookuptable.unlvrtm.nc
```

Gaseous absorption line position and strength depend on both pressure and temperature. However, you don't need to worry if you perform subsequent simulations for a different atmospheric profile or with different atmospheric layers. The model will search for the cross-section data from a same pressure level (or interpolated from the neighboring pressure levels).

3 Output Files

Once the code runs properly, results will be saved in a single netCDF file, the name of which is *prefix.unlvrtn.nc*, where *prefix* is specified in the *namelist.ini* (Section 2.1.9).

Prior to version 1.4.5, however, you may obtain multiple diagnostic files with each for one spectrum. Before version 1.4.5, the diagnostic files are named as *prefix.LAMDAXXXX.nc*, where *XXXX* is spectrum index. For single spectrum simulation, *XXXX* is *0001*. For multi-spectrum (say 40), one NetCDF file will be generated for each individual spectrum from *0001* to *0040*. Along with the NetCDF output file, up to two ASCII files will be generated with filename of *prefix.LAMDA0001.diaginfo* (and *prefix.diaginfo* if multi-spectrum).

Starting from version 1.4.5, model generates a single diagnostic file in the netCDF format without any *.diaginfo* file. The netCDF file contains various model variables as controlled by the DIAGNOSTIC menu in the file *namelist.ini* (Section 2.1.9). This chapter presents in detail about the content in the diagnostic file and how to use them. In addition, you may also see some additional output text file depending on the model setting and running status. We will mentioned these files at the end of this chapter.

3.1 Output NetCDF file

The variables saved to the netCDF files are controlled by the Diagnostic Menu in *namelist.ini* for different categories. Here we list those variables in below Table 3.2–3.10. The netCDF file also contains a few global attributes (Table 3.1) that could be helpful for quick and generic check on the simulation.

3.2 Other Output files

UNL-VRTM may generates following files to the run folder:

- *VLIDORT_BRDF_Check.log* This file will be generated with messages if BRDF prepared for VLIDORT is problematic.
- *VLIDORT_Execution.log* This file will be generated with messages if VLIDORT running with problem or warnings.

- *vlidort.iop.debug* This file is generated when turning on “Write VLIDORT inputs” in the DEBUG menu (Section 2.1.10).

Table 3.1: List of global attributes of the diagnostic netCDF file.

Attribute	Value	Description
History	Created on ...	File generation date/time
Format	netCDF3/netCDF4	netCDF format version
Model	UNL-VRM	Model name
Version	1.x.x	Model version number
VLIDORT	On/Off	On/off for radiative transfer simulation
Vector	On/Off	If a polarimetric run?
Jacobian	On/Off	If a linearized calculation?
Solar Radiation	On/Off	If including solar source?
Thermal Emission	On/Off	If including thermal emisison?
Aerosol	On/Off	If including aerosol?
Tracegas	On/Off	If including tracegas?
Rayleigh	On/Off	If including Rayleigh scattering?
Surface	Lamb/BRDF	BRDF or Lambertian surface?
Success	Yes/No	If simulation is successful?

Table 3.2: List of dimensions.

Dimension Name	Value	Description
Layer	N_Layers	Number of atmospheric layers
Level	N_Layers+1	Number of atmospheric levels
Spectra	NSpectra	Number of spectrum
Gas	nGas	Number of gas species
SZA	N_Theta0	Number of solar zenith angle
VZA	N_Theta	Number of viewing zenith angle
RAZ	N_Phi	Number of relative azimuth angle
Mode	nMode	Number of aerosol mode
Geo	n_Geom	Number of Sun-viewing geometry
Stokes	n_Stoks	Number of Stokes parameters
LOut	NRecep_Lev	Number of receptor level
PSDPar	3	Number of PSD parameters
ProfPar	2	Number of aerosol profile parameters
Moment	n_Moments	Number of Legendre moments
FMat	6	Number of F-Matrix elements
PAngle	nPAngle	Number of phase function angle
BRDFKernel	N_BRDF	Number of BRDF kernels
LinPar	N_LPPar_Total	Number of atmospheric Jacobian
LinSPar	N_LPPar_Surf	Number of surface Jacobian
GMat	nGMMask	Number of Greek matrix elements
LayerRev	N_Layers	Reversed atmospheric layers
LevelRev	N_Layers+1	Reversed atmospheric levels
Ch6	6,	String character of 6
Ch10	10	String character of 10
Ch30	30	String character of 30
Num2	2	Number of 2
Num3	3	Number of 3
Num5	5	Number of 5

Table 3.3: List of Saved Input Variables (DIAG01).

Variable	Units	Longname
Lamdas	nm	Spectral wavelngth
Wavenum	cm ⁻¹	Spectral frequency
FWHM	nm or cm ⁻¹	Spectral full-width at half-maximum
IAtm	none	Atmosphere type ID
SZA	degree	Solar zenith angle
VZA	degree	View zenith angle
RAZ	degree	Relative azimuthal angle
LOut	#level	Receptor level
SSC	none	Single-scatter correction scenario
S0	none	Solar flux factor
TS	Kelvin	Surface temperature
Gas	none	Tracegas names
GasMW	g mol ⁻¹	Tracegas mole weight
GasSF	none	Tracegas scaling factor
ModeFrc	none	Modal fraction
MR	none	Real-part refractive index
MI	none	Imag-part refractive index
PSDRange	microns	Particle size range
PSDId	none	PSD index
PSDPars	varying	PSD parameters
ProfRange	km	Aerosol vertical extending range
ProfId	none	Aerosol vertical profile type number
ProfPars	varying	Aerosol profile parameters
Ref_MR	none	Referenced real-part refractive index
Ref_MI	none	Referenced imag-part refractive index
Ref_PSDRange	microns	Referenced particle size range
Ref_PSDId	none	Referenced PSD index
Ref_PSDPars	varying	Referenced PSD parameters
LinPar	none	Jacobian names

Table 3.4: List of Atmospheric profile variables (DIAG02).

Variable	Units	Longname
Z	km	Level height
P	hPa	Level pressure
T	Kelvin	Level temperature
LayP	hPa	Layer pressure
LayT	Kelvin	Layer temperature
AirDen	molec cm ⁻³	Air number density
GasMR	ppmv	Gaseous mixing ratio
AerVol	micron ³ micron ⁻²	Aerosol volume profile
AerNum	micron ⁻²	Aerosol number profile

Table 3.5: List of Aerosol Scattering Quantities (DIAG03).

Variable	Units	Longname
PAngle	Degree	Equidistant scattering angles 1. Extinction cross-section 2. Scattering cross-section 3. Single scattering albedo 4. Extinction efficiency 5. Scattering efficiency
Bulk_AOP	varying	Mie/Tmatrix bulk parameters
Asymm	none	Asymmetric factor
Dist	varying	Size distribution parameters 1. Number Density (normalized to1) 2. Cross-section 3. Volume 4. Effective radius 5. Effective variance
ExpCoeffs	none	Greek matrix expansion coefficients
FMatrix	none	Scattering F-matrix (F11, F33, F12, F34)
LPSD_Bulk	varying	Bulk_AOP derivatives wrt PSD
LPSD_Dist	varying	PSDPars derivatives wrt PSD
LPSD_FMatrix	varying	FMatrix derivatives wrt PSD
LRFE_Bulk	varying	Bulk_AOP derivatives wrt refractive index
LRFE_FMatrix	none	FMatrix derivatives wrt refractive index
LFrc_Bulk	varying	Bulk_AOP derivatives wrt modal fraction

Table 3.6: List of Atmospheric optical profiles (DIAG04).

Variable	Units	Longname
Xsec_SAO	$\text{cm}^2 \text{ molec}^{-1}$	Gas-absorption cross-section (SAO)
Xsec_LBL	$\text{cm}^2 \text{ molec}^{-1}$	Gas-absorption cross-section (HITRAN)
Xsec_Combined	$\text{cm}^2 \text{ molec}^{-1}$	Gas-absorption cross-section combined
tauGas_SAO	none	Gas-absorption optical depth (SAO)
tauGas_LBL	none	Gas-absorption optical depth (HITRAN)
tauGas_Combined	none	Gas-absorption optical depth combined
tauGas	none	Bulk gas-absorption optical depth
tauRayleigh	none	Rayleigh-scattering optical depth
Rayleigh_FMatrix	none	Rayleigh-scattering Greek matrix
tauAER	none	Aerosol optical depth
omegaAER	none	Aerosol single scattering albedo

Table 3.7: List of Surface optical variables (DIAG05).

Variable	Units	Longname
Lamb_Albedo	none	Lambertian albedo
BRDFKernel	none	BRDF kernel names
BRDFFactor	none	BRDF coefficients
BRDFVal	none	Exact direct BRDF values
SLeaveVal	none	Isotropic surface-leaving radiance

Table 3.8: List of VLIDORT Inputs Variables (DIAG06).

Variable	Units	Longname
GMat	none	Masking index for Greek matrix
tauIOP	none	Bulk atmospheric optical depth
omegaIOP	none	Bulk atmospheric single scattering albedo
GMatIOP	none	Bulk atmospheric scattering Greek matrix
tauLIOP	none	tauIOP linearized inputs
omegaLIOP	none	omegaIOP linearized inputs
GMatLIOP	none	GMatIOP linearized inputs

Table 3.9: List of Radiative transfer variables (DIAG07).

Variable	Units	Longname
Geo_Offset	none	VZA offset
Stokes	none	Stokes vector
Mean_Stokes	none	Stokes mean vector (actinic flux)
Flux_Stokes	none	Stokes flux vector (regular flux)
Mean_Direct	none	Stokes direct mean vector (actinic flux)
Flux_Direct	none	Stokes direct flux vector (regular flux)
Emiss_Surface	W/m ² /sr/um or W/m ² /sr/cm ⁻¹	Surface thermal emission
GDT_Emiss_Surface	W/m ² /sr/um/K or W/m ² /sr/cm ⁻¹ /K	Gradient Emiss_Surface wrt surface T
Emiss_Atmos	W/m ² /sr/um or W/m ² /sr/cm ⁻¹	Air thermal emission
GDT_Emiss_Atmos	W/m ² /sr/um/K or W/m ² /sr/cm ⁻¹ /K	Gradient Eimss_Atmos wrt air T

Table 3.10: List of VLIDORT Jacobian variables (DIAG08).

Variable	Units	Longname
Jacob_Column	varying	Columnar Jacobians
Jacob_Prof	varying	Profile Jacobians
tauAER_WFS	varying	AOD profile Jacobians
Jacob_Surface	varying	Surface Jacobians

4 For Advanced Users

4.1 Run UNL-VRM beyond the *namelist.ini* file

To be filled

4.2 Making code modifications

To be filled

5 The Useful IDL/Python Programs

There are a few IDL codes in the *util* folder for reading and processing the model results.

More detail to be filled here ...