

User's Guide for UNL–VRTM

A UNified Linearized Vector Radiative Transfer Model

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<http://www.unl-vrtm.com>

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Recent UNL-VRTM Versions

| Version | Date | git ID | Remark |
|---------|-------------|---------|--|
| 1.6.2 | 01 Jul 2017 | d640317 | Bug fix on spectral convolution; change aerosol loading input |
| 1.6.1 | 05 May 2017 | 4124c80 | HITRAN2012 is now included for major gases |
| 1.6.0 | 25 Apr 2017 | eea6a62 | Continuum absorption added for water vapor, CO ₂ , O ₃ , O ₂ and N ₂ . |
| 1.5.3 | 12 Apr 2017 | 605fea9 | Option for user-specified surface pressure and altitude |
| 1.5.2 | 26 Oct 2016 | b4e7de2 | Weighting function for individual gas; redefine azimuth angles; gas spectral convolution on transmittance |
| 1.5.1 | 13 Sep 2016 | 77a9842 | Option for profile and/or column Jacobians; |
| 1.5.0 | 11 Jul 2016 | e880e46 | GEOS5 profile; User aerosol profile; single scattering property without Mie; gas transmittance |
| 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 v1.6.2

- Bug fix for spectral convolution of gas absorption when frequency as input.
- Modify the namelist input for aerosol loading, now specifies loading of each mode. Previous versions specify total loading and modal fraction.
- To check the code update with Git:

```
git diff --name-status 4124c80 d640317
```

New in v1.6.1

- HITRAN 2012 added for major trace gases.
- Gas transmission is validated against MODTRAN for spectral region 0.8 - 2.1 um with the help of Xiuhon Chen (U. Michigan)
- To check the code update with Git:

```
git diff --name-status eaa6a62 4124c80
```

New in v1.6.0

- Continuum absorption is now implemented for water vapor, CO₂, O₃, O₂ and N₂. The continuum code was provided by Vijay and based on AER's MT_CKD version 2.8. Calculated water vapor continuum transmission was validated against MODTRAN simulation provided by Xiuhong Chen.
- Option to turn on/off HITRAN, SAO, and continuum absorption is now included in the namelist file.

- To check the code update with Git:

```
git diff --name-status 605fea9 eaa6a62
```

New in v1.5.3

- Add option for user-specified surface pressure and altitude
- Remove folder doc, so now user guide is a standalone repository
- To check the code update with Git:

```
git diff --name-status b4e7de2 605fea9
```

New in v1.5.2

- Add output of weighting function for individual gas
- Update compile/Makefile scripts for easily compile options
- Now the azimuth angles is redefined to be same as MODIS level-1 data definition
- Now the spectral convolution of HITRAN absorption line is in terms of transmittance
- To check the code update with Git:

```
git diff --name-status 77a9842 b4e7de2
```

New in v1.5.1

- Add option for profile and/or column Jacobians in namelist.ini.
- To check the code update with Git:

```
git diff --name-status e880e46 77a9842
```

New in v1.5.0

- User input Z, P, T, and aerosol extinction profile, gaseous mixing ratio with a netcdf file is not fully verified (feature developed specifically for DSCOVR project).
- A specific 47-layer profile (IATM = -47) is added. This profile is defined following GEOS-5 reduced vertical grid (47 hybrid pressure-sigma levels).
- Option to specify gaseous loading in terms of transmittance: set a negative value (= -transmittance) in the scaling factor column of the corresponding gas(es).
- Option to specify single scattering albedo and phase function directly with an input file *aerosol_M0X.dat* (where X = 1 or 2 indicating aerosol mode).
- To check the code update with Git:

```
git diff --name-status e6f25f8 e880e46
```

New in v1.4.6

- User-specified atmospheric profile is now enabled. The model could read height and pressure grid, air temperature and gaseous profiles from a well-prepared text file (atmos.dat, efforts ongoing) 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-VRM

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 (1) **create an account on <https://gitlab.com>** and (2) **tell me your username**. I will add you as a member of the UNL-VRM 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-VRM 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/unl-vrtm.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:

```
README run/ src/
```

A short description of each subdirectory is as following:

- 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.

Other directories (*doc/* and *util/*) might exist for versions prior to 1.6, which contained User's Guide and some IDL analysis codes. User's Guide is now a standalone repository at [GitLab](https://gitlab.com/unl-vrtm) and is published at <http://www.unl-vrtm.com/doc/>. A python module for processing UNL-VRM is now under development and will be released in the near future.

1.3 Compile UNL-VRM

Here are some know requirements for the compilation of UNL-VRM:

- Hardware: Intel machine with RAM of 2GB or more.
- Operation system: Linux OS on single platform or clusters.
- Dependencies: (1) Fortran 90/95 (known to work with ifort 12 and newer); (2) NetCDF for Intel Fortran (version 4.2 and newer); (3) A 'make' command

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-VRMall and all of the necessary libraries.

Later if you made revisions about the codes but not the libraries, you could compile UNL-VRM 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.

(new in v1.5.2) Now executing the file *compile* will prompt a few options for compilation including full, quick, and debug option, etc.

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 Obtaining Ancillary Data

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.

These ancillary data can be downloaded from <http://www.unl-vrtm.com/download/>.

- For version 1.3.x: [data.1.3.tar](#)

- For version 1.4.x: [data.1.4.x.tar](#)
- For version 1.5.x: [data.1.5.x.tar](#)
- For version 1.6.x: [data.1.6.x.tar](#)

1.5 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 different type of shell (like csh) on your machine.

2 Input Files

This chapter describe 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 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  - number of layers    : -1
8  - surf altitude (m)   : -1
9  - surf pressure (hPa) : 950.0
10 Run  directory       : ./
11 Data  directory      : /work/jwang7/xxu/ARTDATA/data/
12 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 Gassian-shape spectral reponse.

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 (new v1.4.6)
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.
- -47: GEOS-5 reduced vertical grid with 47 hybrid pressure-sigma levels. (new v1.5.0)

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 surface altitude in meter. Default is -1 with no adjustment for atmospheric profile. If a positive number is given, atmospheric profile will be adjusted based on the surface altitude.
9. Specifies surface pressure in hPa. Default is -1 with no adjustment for atmospheric profile. If a positive number is given, atmospheric profile will be adjusted based on the surface pressure.
10. Specifies the model run directory. Generally, it is `"/` which indicates the current directory.
11. Specifies the directory where the ancillary data is placed.
12. 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 hhmmss    : 20120101 103000
6   - latitude longitude  : 10 -20
7 View zenith angle(s)    : 0
8 View azimuthal angle(s) : 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.

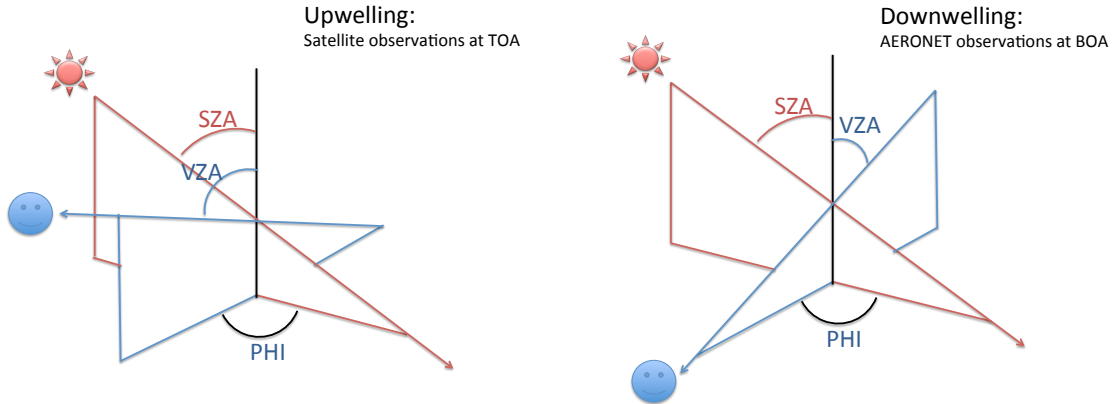


Figure 1: Illustration of UNL-VRTM geometry. SZA: solar zenith angle, VZA: viewing zenith angle, PHI: relative azimuth angle.

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 hhmmss.
6. Specifies the latitude and longitude of the observing location in degree.
7. Specifies viewer zenith angles. You may list one or more (up to 4) values.
8. Specifies the viewer 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.

Here, solar and viewing zenith angles are defined as the angle of their positions to the vertical at observing target, i.e., 0° when directly overhead, and 90° when in the horizon. Solar and viewing azimuth angles are defined clockwise from due north, i.e., north is 0° , east is 90° , south is 180° , and west is 270° . These definitions are the same to those used in MODIS level-1 geolocation products. (new in v1.5.2)

VLIDORT only requires a relative azimuth angle, which is calculated from the input solar and view azimuth angles based on the light beam directions. Solar beam

has a sun-to-target direction, while light beam to the viewer (sensor) is from-target-to-sensor. So, the relative azimuth angle is the angle between directional target-to-sun plane and target-to-sensor plane. Since the relative azimuth angle is based on light beam direction, its calculation is different between a satellite sensor and a ground-based sensor (like AERONET sun photometer). See Figure 1 for illustrations.

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 Profile Jacob.?  : T
3  Turn on Column Jacob.?   : T
4   - wrt Gas?              : F
5   - wrt AOD?              : F
6   - wrt SSA?              : F
7   - wrt aerosol volume?   : T
8   - wrt mode fraction?    : F
9   - wrt refractivity?     : T
10  - wrt shape factor?     : F
11  - wrt size dist?        : T
12  - wrt aerosol profile?:  F
13  Non-varying volume?     : T
14  Non-varying AOD?        : F
15  Turn on surface Jacob.?  : T
16   - wrt BRDF factor?     : T
17   - wrt BRDF parameter?  : F
18  Do FD verication?      : F

```

Description:

1. Title for Jacobian menu.
2. Switch to turn on/off the calculation for **profile** Jacobian for atmospheric trace gas or aerosol parameters.
3. Switch to turn on/off the calculation for **columnar** Jacobian for atmospheric trace gas or aerosol parameters.
If both column and profile Jacobian set false, all the atmospheric Jacobian calculations will be turned off. (Profile/column option new for version 1.5.1)
4. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to total gas absorption optical depth.
5. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol optical depth.
6. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol single scattering albedo.
7. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol volume.
8. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol modal fraction.
9. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol refractive indices.
10. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol shape factor (with T-Matrix code turned on).
11. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol size distribution parameters.
12. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to aerosol vertical profile parameters.
13. If true, keep the mass constant (but varying AOD) in the Jacobian calculation.
14. 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.

15. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to surface reflectance.
16. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to BRDF amplitude factor of each kernel.
17. Switch to turn on/off the calculation of Jaocbian of Stokes components with respect to BRDF kernel parameters.
18. 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

```

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 |

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 (available in 0.40–14.01 μm)
 - 3: sea-water surface (available in 2.08–14.01 μm)
 - 4: fine-snow surface (available in 0.30–14.01 μm)
 - 5: medium-snow surface (available in 0.30–14.01 μm)
 - 6: surface with deciduous trees (available in 0.30–14.01 μm)
 - 7: surface with green grasses (available in 0.30–14.00 μm)
 - 8: surface with gry grasses (available in 0.38–14.00 μm)
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  Columnar loading(s)       : 0.2      0.3
5  - is AOD?                 : T
6  - is Vol (um3/um2)?      : T

```

```

7 Mie/T-Mat/User (1/2/-1) : 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 aerosol loading of each mode, i.e., one number for single mode and two for bimode (modified v1.6.2, previously, it specifies modal fraction). Note that these could be either AOD or aerosol volume, depending on which is used as loading input in the following two lines.
5. Turn on/off using column AOD as aerosol loading inputs.

6. Turn on/off using columnar volume as aerosol loading inputs. 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.
From version 1.5.0, use can directly specify single scattering albedo and phase function (**set -1**), rather than from the Mie/T-Matrix calculation. Then, user will need to place a text file in the run folder with name *aerosol.M01.dat* and/or *aerosol.M02.dat* for the first and/or second aerosol mode, respectively. Example file can be found in the *run* folder of standard model package. User can set -1 for either one of the two modes or both modes. However, direct input of SSA and phase function will not allow the Jacobian calculation to aerosol size, refractive index, and shape. See section 2.4 on how to prepare the file for aerosol single scattering albedo and phase function.
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. This line reads two variables: NP and EPS. NP indicates non-spherical type, while EPS is a aspect ratio or deformation parameter. For spheroids NP=-1 and EPS is the ratio of the horizontal to rotational axes. EPS is larger than 1 for oblate spheroids and smaller than 1 for prolate spheroids. For cylinders NP=-2 and EPS is the ratio of the diameter to the length. For Chebyshev particles NP must be positive and is the degree of the Chebyshev polynomial, while EPS is the deformation parameter.
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

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 |

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.
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
```


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 |

```

3 Use pre-calculated data?: T
4 - give the data file : clarreo.unlvrtm.nc
5 Include HITRAN lines? : T
6 Include SAO UV-Vis xsec?: T
7 Include continuum? : T
8 Num. of trace gases : 22
9 Trace gas Entries ==> : TR# Name M-Weight Include? Scaling
10 Trace gas #1 : 1 H2O 18.015 T 0.15
11 Trace gas #2 : 2 CO2 44.010 T 1.0
12 Trace gas #3 : 3 O3 47.998 T 1.25
13 Trace gas #4 : 4 N2O 44.010 T 1.0
14 Trace gas #5 : 5 CO 28.011 T 1.0
15 Trace gas #6 : 6 CH4 16.043 T 1.0
16 Trace gas #7 : 7 O2 31.999 T 1.0
17 Trace gas #8 : 8 NO 30.010 T 1.0
18 Trace gas #9 : 9 SO2 64.060 T 1.8
19 Trace gas #10 : 10 NO2 46.010 T 1.8
20 Trace gas #11 : 11 NH3 17.030 F 1.0
21 Trace gas #12 : 12 HNO3 63.010 F 1.0
22 Trace gas #13 : 13 OH 17.000 T 1.0
23 Trace gas #14 : 14 HF 20.010 F 1.0
24 Trace gas #15 : 15 HCL 36.460 F 1.0
25 Trace gas #16 : 16 HBR 80.920 F 1.0
26 Trace gas #17 : 17 HI 127.91 F 1.0
27 Trace gas #18 : 18 CLO 51.450 F 1.0
28 Trace gas #19 : 19 OCS 60.080 F 1.0
29 Trace gas #20 : 20 H2CO 30.030 T 1.0
30 Trace gas #21 : 21 HOCL 52.460 F 1.0
31 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 2.5 for a detail description of this option.
4. Specifies the netCDF filename that contains pre-cauclated gas cross-sections, if True for the Use of pre-calculated data.
5. Switch to turn on/off gas absorption from HITRAN database. Recommend to turn on for a realistic simulation.
6. Switch to turn on/off gas absorption from SAO UV-vis cross-section database. Recommend to turn on for a realistic simulation.
7. Switch to turn on/off gas continuum absorption using CKD model. Recommend to turn on for a realistic simulation.
8. Specifies the total number of considered trace gas. This **must** be 22 in the current version of the model.
9. Entries.
10. 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.
New in v1.5.0: In the scaling column, user can set a negative transimttane value for any gases. The model will scale the columnar concentration of the corresponding gases according to the transmittance.

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  : cnt1
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 factors for each kernel specified in the *namelist.ini* will also be replaced.
- If Lambertian surface is considered, a "-1" must be 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 reflectance: -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.

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.

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 |

- 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 Optional optical property file: *aerosol_M0X.dat*

New in v1.5.0. To directly read aerosol single scattering albedo (SSA) and phase function set `-1` at below line in the namelist file:

```

%% AEROSOL MENU %%      :
.....
Mie/T-Mat/User (1/2/-1) : -1      -1

```

You can set `-1` for one of the two modes or for both modes. The model then reads the data from *aerosol_M01.dat* and/or *aerosol_M02.dat*, with M01 for the first mode and M02 for the second. The SSA and phase function will be applied for all layers. The file can be prepared following:

- First line is title line, you can put any words in.
- Second line is SSA value in floating point format.

- In the following lines, a scattering angle value and a phase function value are placed in each line. **Currently we fix the number of scattering as 83, as defined in AERONET inversion product. Later will be updated to add flexibility.**

2.5 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.unlvrtm.nc*, where *prefix* is specified in the *emphnamelist.ini* (Section 2.1.9).

Prior to version 1.4.5, however, you should 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_LPar_Total | Number of atmospheric Jacobian |
| LinSPar | N_LPar_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 |
| ZS | m | Surface altitude (new v1.5.3) |
| PS | hPa | Surface pressure (new v1.5.3) |
| SZA | degree | Solar zenith angle |
| VZA | degree | View zenith angle |
| RAZ | degree | Relative azimuthal angle (see Fig. 1) |
| LOut | #level | Recptor 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 (GK-matrix indexing: 11, 22, 33, 44, -12, 34) |
| FMatrix | none | Scattering F-matrix (F-matrix indexing: 11, 12, 22, 33, 34, 44) |
| 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 | cm ² molec ⁻¹ | Gas-absorption cross-section (SAO) |
| Xsec_LBL | cm ² molec ⁻¹ | Gas-absorption cross-section (HITRAN) |
| Xsec_CTN | cm ² molec ⁻¹ | Gas-absorption cross-section (Continuum), new v1.6.0 |
| Xsec_Combined | cm ² molec ⁻¹ | Gas-absorption cross-section combined |
| tauGas_SAO | none | Gas-absorption optical depth (SAO) |
| tauGas_LBL | none | Gas-absorption optical depth (HITRAN) |
| tauGas_CTN | none | Gas-absorption optical depth (Continuum), new v1.6.0 |
| 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 |

Note: For these variables, the dimension for atmospheric layer starts from top layer and ends at bottom layer.

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/m2/sr/um or W/m2/sr/cm ⁻¹ | Surface thermal emission |
| GDT_Emiss_Surface | W/m2/sr/um/K or W/m2/sr/cm ⁻¹ /K | Gradient Emiss_Surface wrt surface T |
| Emiss_Atmos | W/m2/sr/um or W/m2/sr/cm ⁻¹ | Air thermal emission |
| GDT_Emiss_Atmos | W/m2/sr/um/K or W/m2/sr/cm ⁻¹ /K | Gradient Eimss_Atmos wrt air T |

Note: If thermal calculation turned off, Stokes is unitsless because it is a normalized quantity; if thermal calculation turned on, its units should be (W/m2/sr/um) or (W/m2/sr/cm⁻¹) depending on wavelength or frequency as the model input.

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

| Variable | Units | Longname |
|----------------|----------------|-----------------------|
| Jacob_Column | same to Stokes | Columnar Jacobians |
| Jacob_Prof | same to Stokes | Profile Jacobians |
| Jacob_Prof_Gas | same to Stokes | Gas profile Jacobians |
| tauAER_WFS | same to Stokes | AOD profile Jacobians |
| Jacob_Surface | same to Stokes | Surface Jacobians |

Note: Jacobian is defined as $x \frac{\partial S}{\partial x}$ for all above variables except Jacob_Surface. Jacob_Surface is defined as $\frac{\partial S}{\partial x}$. Here, S is the Stokes vector, x is the weighting function denominator. For profile Jacobian variables, the dimension for atmospheric layer starts from top layer and ends at bottom layer.

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 ...