

User's Guide for UNL–VRTM

A UNified Linearized Vector Radiative Transfer Model

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<https://unl-vrtm.org>

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Recent Updates

UNL-VRM Versions

Version	Date	git ID	Remark
2.1.8	12 Dec 2019	077c7a5	BPDF corrected; 2-level radiance output enabled; max spectra increased to 50K; compiled with ifort 13.1.3
2.0.1	26 Sep 2018	3d44670	Version with pre-compiled static libraries
1.6.4	15 Feb 2018	fad6742	Improvement in gas LBL and continuum absorpton; inclusion of scattering for shortwave IR calculation
1.6.3	19 Dec 2017	07f7558	Minor upgrades on makefiles, code remains same to v1.6.2.
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

New in v2.1.8

- Previously incorrect BPDF treatments for Giss-Cox-Munk and BPDF2009 kernels are fixed (detailed inputs for BRDF/BPDF are introduced in Sec 2.1.5 of User's Guide)
- Radiation fields can be outputted for 2 different atmospheric levels
- Maximum number of spectra is increased to 50000 to allow super hyperspectral simulation
- Relative azimuth angle is now in range 0 - 360 degrees (previously 0 - 180)
- Minor bugs fix for gases LUT reading; surface elevation input, F-matrix ordering, and PPCO2 for Rayleigh etc

New in v2.0.1

- Re-organized package structure
- Core codes are pre-compiled into libraries
- Version control with Git was disabled

New in v1.6.4

- Update README.md file
- Bug fix for the overflow issue in HIRATN spectral convolution (reported by Xiuhong)
- Update transonly option for thermal
- Fixed the issue for incorrect surface gas mixing ratio for user-specified surface pressure
- Bug fixes for continuum absorption

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 DSCOVOR 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 gasous 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 gasesou 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 subsquent 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.

Use this list to see if an issue affecting you is already known and decide when to upgrade. Fixed issues are removed after a major version update (e.g., 1.5.x to 1.6.x).

Jacobian spikes

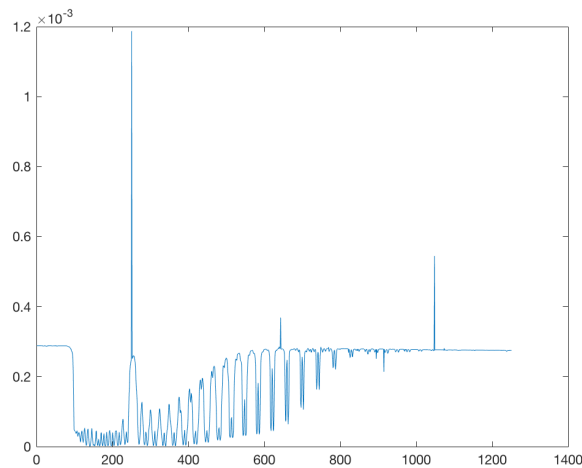


Figure 1: An example of Jacobian spikes. X and Y axes represent spectral index and Jacobian, respectively. The Jacobian is of TOA intensity with respect to fine-mode aerosol volume. The spectral range is 758–778 nm around the oxygen-A band, with spectral resolution and interval of 0.04 and 0.016 nm, respectively.

Erroneous Jacobian with atmospheric parameters (aerosol, cloud, or gas) could be encountered randomly. It often occurs in the hyperspectral simulations, especially when hundreds or thousands of spectra are considered, where Jacobian spikes may take place over several spectral samplings. Figure 1 gives an example of Jacobian spikes. Those Jacobian spikes are caused by incorrect Jacobian calculation at certain atmospheric level, which is possibly related to mathematic issue during the Fourier expansion and integral in solving the radiative transfer equation.

A practical solution for this issue is a smoothness examination in the post-processing.

1 Getting Start

1.1 Obtaining the UNL-VRTM

Model packages including source code and core libraries are available upon request. The request can be made on <https://unl-vrtm.org>. Our support team will provide FTP access to model and data package within 3 business days of receipt of the request.

1.2 Directory Structure Overview

The model package is named as `unl-vrtm-x.x.x-ifort-y.y.y-gitzzzzzzz.tar`, where `x.x.x` is the version of UNL-VRTM model, `ifort-y.y.y` is the version of the Intel Fortran compiler that was used to compile the model's core codes into libraries, and `gitzzzzzzz` is the git ID of core source codes. Unzip this tar package will generate a folder `unl-vrtm-x.x.x` that consists of several subdirectories. A `ls` command should give you:

```
LICENSE.txt  README.md  build*  mods/  run/  src/
```

A short description of each subdirectory is as following:

- `LICENSE.txt`: The UNL-VRTM MIT License agreement.
- `README.md`: The readme file, where basic information of UNL-VRTM and instructions of how to compile the model can be found.
- `build*`: An executable bash script to compile UNL-VRTM. This is the file that requires user to specify run folder and set environment variables for netcdf and/or fortran compiler.
- `mods/`: Folder to carry compiled libraries of UNL-VRTM core codes. Usually, there is no need to bother this folder.
- `src/`: Folder to carry several uncompiled source codes.
- `run/`: Run folder used to run the model, which contains necessary namelist file and input files.

1.3 Requirements

Here are some known requirements for compiling and running UNL-VRTM:

- Hardware: Intel machine with RAM of 2GB or more.
- Operation system: Linux OS on a single platform or clusters. A MacOS version under development.
- Compiler: Fortran 90/95 (known to work with ifort YY.Y.Y and newer); a gfortran version is under development.
- NetCDF version 4.2+ installed and linked to the Fortran compiler.
- GUN Make command.

1.4 Compile UNL-VRTM

A full compilation is necessary when you first get the codes. It is done by executing the file `build*` in main folder. However, it should be noted that

- Always use the Intel Fortran compiler of the version as indicated in the `unl-vrtm` package filename. Use other Fortran compiler or a different version of ifort will likely result in compiling errors.
- Have NetCDF version 4.2 or newer installed along with the Intel Fortran.
- Set the environment variable of `NETCDF_PATH` in `build*`.
- Specify the target directory for UNL-VRTM executive, `unl-vrtm.exe`. Once the compilation succeeds, `unl-vrtm.exe` will be generated in the specified directory.

1.5 Obtaining Ancillary Data

In addition, the model needs a set of ancillary data, including the gaseous spectroscopic line parameters and cross section database, which are stored in a `data/` folder. The path for the `data/` folder needs to be specified in the model input file. Users should obtain the data access along with the code access. If not, these data can also be downloaded from <http://www.unl-vrtm.com/download/>, which contains the data package for various model versions:

- For `unl-vrtm 1.3.x`: `data.1.3.tar`

- For unl-vrtm 1.4.x: `data.1.4.x.tar`
- For unl-vrtm 1.5.x: `data.1.4.x.tar`
- For unl-vrtm 1.6.x: `data.1.6.x.tar`
- For unl-vrtm 2.0.x: `data.2.0.x.tar`

1.6 Run UNL-VRTM

Upon compilation, `unl-vrtm.exe` will be generated in the specified run folder, where this file will be executed to run UNL-VRTM simulations. Of course, user can also move or copy the `unl-vrtm.exe` file to a different run folder and perform simulations. The model run needs an input file `namelist.ini` that specifies the settings for the simulation. 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 (i.e., by executing `./unlvrtm.exe`), 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
```

Please note that 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 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  - 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 - yyyymmdd 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 ONE single solar zenith angle.

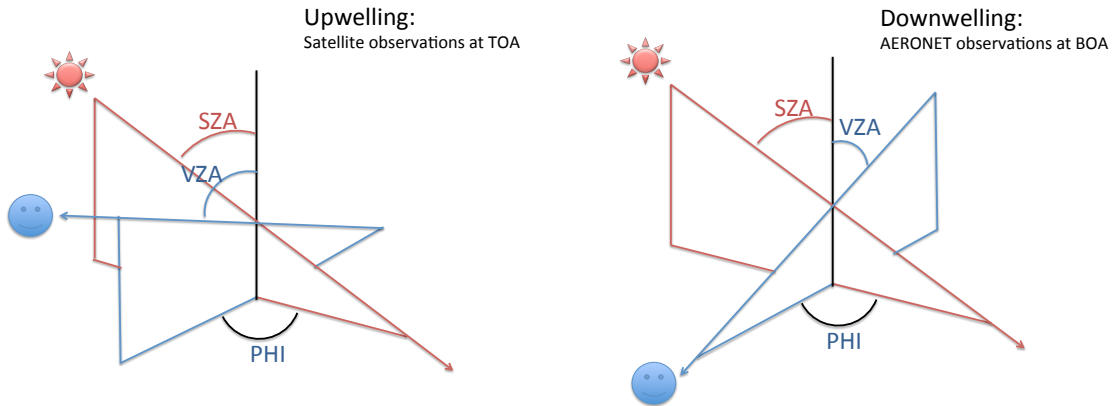


Figure 2: Illustration of UNL-VRTM geometry. SZA: solar zenith angle, VZA: viewing zenith angle, PHI: relative azimuth angle.

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 10) values.
8. Specifies the viewer azimuth angles, number of which is 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 same to those used in MODIS level-1 geolocation products. (new in v1.5.2)

VLIDORT requires the input of 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 sun-to-target 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 2 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, max=15
5. Specifies number of Legendre expansion terms for Greek Matrix. Current maximum is 180, but it can be increased in an extended version.
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 verification?     : 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 and must one of this and above one should be true.
15. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to surface reflectance.
16. Switch to turn on/off the calculation of Jacobian of Stokes components with respect to BRDF amplitude factor of each kernel.
17. Switch to turn on/off the calculation of Jacobian 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 reflectance:    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`

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	Wanner et al., 1995
4	Li-sparse	2	Scalar	Wanner et al., 1995
5	Li-dense	2	Scalar	Wanner et al., 1995
6	Hapke	3	Scalar	Hapke, 1993
7	Roujean	0	Scalar	Wanner et al., 1995
8	Rahman(RPV)	3	Scalar	Rahman et al., 1993
9	Cox-Munk	2	Scalar	Cox & Munk, 1954
10	GissCoxMnk	2	Vector	Mishchenko & Travis 1997
11	GCMcomplex	3	Vector	GissCoxMnk + complex RI
12	BPDF2009	2	Vector	Maignan et al., 2009

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 dry 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 and their required parameters).

On Kernel Parameters: The following kernels require user to specify relevant parameters. Details on the kernel functions are presented in Xu and Wang (2019) "UNL-VRM: a testbed for aerosol remote sensing: Model developments and Applications". Below lists those required parameters and corresponding source equations from the above reference.

- Li-sparse and Li-dense kernel: 2 parameters are crown ratio b/r and height ratio h/b , see Eq. (106-112) in Xu and Wang (2019)
- Hapke kernel: 3 parameters are single scattering albedo ω , amplitude B_0 , and angular width (h) of the hot spot, see Eq. (113-115) in Xu and Wang (2019)
- Rahman (RPV) kernel: 3 parameters are amplitude parameter ρ_0 , the Henyey-Greenstein phase function g , and k for characterizing angular spread, see Eq. (118-119) in Xu and Wang (2019)
- Cox-Munk kernel: 2 parameters are geometric factor σ^2 and square of water refractive index m^2 , σ^2 is related to wind speed w by $\sigma^2 = 0.003 + 0.00152w$, see Eq. (128-129) in Xu and Wang (2019)
- GissCoxMunk kernel: vector form of Cox-Munk with 2 different parameters, half of geometric factor $0.5\sigma^2$ and refractive index m
- GCMcomplex kernel: similar to GissCoxMunk kernel but considering the absorption of the water surface. 3 parameters are geometric factor σ^2 , real and imaginary parts of water refractive index BPDF2009 (Maignan) kernel: 1 parameter is the NDVI ν , see Eq. (120-127) in Xu and Wang (2019)

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
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].

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

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: $\tau(z) = K \frac{\exp(-\gamma|z-z_{peak}|)}{[1+\exp(-\gamma|z-z_{peak}|)]^2}$, where K is related to the columnar loading, z_{peak} is the height where modal aerosol extinction peaks, and γ is related to the width σ by $\gamma = \frac{\ln(3+\sqrt{8})}{\sigma}$.
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 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 transmittance 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  : 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 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` or `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 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
DIAG01: Model inputs     : T
DIAG02: Atmos profiles   : T
.....
DIAG04: Optic profiles   : T
.....
```

This simulation will yield a diagnostic file (`lbl-lookuptable.unlvrtm.nc`) according to above settings (Note: DIAG01, DIAG02, and DIAG04 have to be turned for generating this LUT file).

- 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 `namelist.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. 2)
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
Bulk_AOP	micron ⁻²	Mie/Tmatrix bulk parameters:
	micron ⁻²	1. Extinction cross section
	none	2. Scattering cross section
	none	3. Single scattering albedo
	none	4. Extinction efficiency
	none	5. Scattering efficiency
Asymm	none	Asymmetric factor
Dist		Size distribution parameters:
	micron ⁻²	1. Number Density (normalized to 1)
	micron ³	2. Geometric cross section
	micron	3. Volume
	none	4. Effective radius
	none	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 total flux)
Flux_Stokes	none	Stokes flux vector (regular total flux)
Mean_Direct	none	Stokes direct mean vector (actinic direct flux)
Flux_Direct	none	Stokes direct flux vector (regular direct 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 ...