

Frequently Asked Questions about LNFL and LBLRTM AER, Inc.

1	FAQ Questions – (click on section number for direct link).....	2
2	General LBLRTM Description	3
3	General LNFL/LBLRTM File Information	3
3.1	Platforms on which LBLRTM can be run	3
3.2	Issues relating to unformatted files on UNIX and LINUX systems	4
3.3	LNFL/LBLRTM Naming Convention.....	4
3.4	LNFL/LBLRTM Input File (TAPE5) Format	4
3.5	LBLRTM Output File Format	5
4	Instructions and Tips for Running LNFL	5
4.1	Input files for LNFL.....	5
4.2	Output files for LNFL	5
4.3	Sequence for running LNFL	6
5	Instructions and Tips for Compiling and Running LBLRTM	6
5.1	Required input files for LBLRTM.....	6
5.2	Layer numbering scheme.....	6
5.3	Output files for LBLRTM.....	6
5.4	Sequence for running LBLRTM.....	7
6	General Questions.....	7
6.1	What is the difference between a line-by-line calculation and a band-model calculation?	7
6.2	What are the standard units used in LBLRTM calculations?	7
6.3	Radiance Derivatives (Jacobians)	8
6.4	Does LBLRTM include heavy molecule parameters (cross-sectional species)?	10
6.5	Format of external surface emissivity/reflectivity files	10
6.6	Absorption due to clouds/aerosols and LOWTRAN5 routines	11
6.7	Solar Radiance	11
6.8	Line coupling	11
6.9	What is the appropriate reference for LBLRTM calculations in journal articles and presentations?.....	12
6.10	How do you calculate fluxes?	12

DRAFT

1 FAQ Questions – (click on section number for direct link)

What is LNFL? 2

What is LBLRTM? 2

Is there a published reference? 6.9

What is the difference between a line-by-line model and a band model? 6.1

What input files are required for LBLRTM? 5.1

What input files are required for LNFL? 4.1

How do I obtain the HITRAN database? 2

What output files are generated by LNFL? 4.2

What output files are generated by LBLRTM? 5.3

What is the structure of the unformatted output files? 3.5

What is the structure of the TAPE5 file? 3.3

Do I need to fill in all of the TAPE5 parameters? 3.3

How do I perform calculations of radiance derivatives (jacobians)? 6.2

Issues relating to unformatted files on UNIX and LINUX systems 3.2

How do I include heavy molecules not included on HITRAN (CFCs, etc.)? 6.4

What is the format of external surface emissivity and/or reflectivity data files? 6.5

How can absorption due to clouds and aerosols be included in the calculation? 6.6

What is the LOWTRAN part of LBLRTM? 6.6

Is there an example run file available? 3

What is the layer numbering scheme? 5.2

How do I include the solar radiance in my calculation? 6.7

What is line coupling and why do I care? 6.8

Are there any restrictions on the bandwidth for a given run? 5

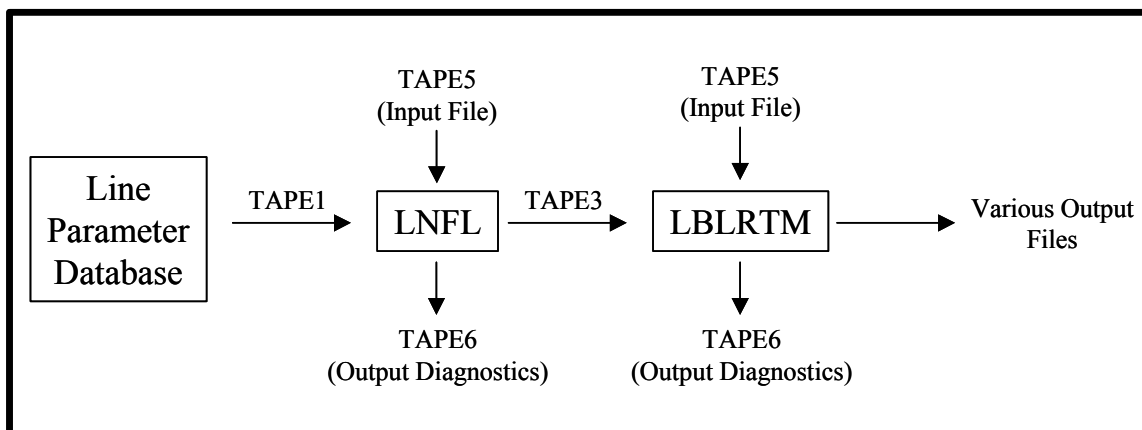
On what platforms can I run LNFL/LBLRTM? Will it run on Windows? 3.1

How do you calculate fluxes? 6.10

2 General LBLRTM Description

LBLRTM (Line-By-Line Radiative Transfer Model) is an accurate and efficient line-by-line radiative transfer model derived from the Fast Atmospheric Signature Code (FASCODE). LBLRTM has been, and continues to be, extensively validated against atmospheric radiance spectra from the ultraviolet to the sub-millimeter.

The HITRAN database (<http://cfa-www.harvard.edu/hitran>) provides the basis for the line parameters used in LBLRTM. These line parameters, as well as additional line parameters from other sources, are extracted for use in LBLRTM by a line file creation program called LNFL. A line parameter database built from HITRAN and suitable for use with LNFL is available from the AER RT web site (rtweb.aer.com).



3 General LNFL/LBLRTM File Information

3.1 Platforms on which LBLRTM can be run

It is recommended that LNFL and LBLRTM be compiled in Fortran 90.

Table 1. Current LBLRTM platforms.

System	Manufacturer	Compiler	Single	Double
IRIX	SGI		F90, f77	F90, f77
SOLARIS	SUN		F90, f77	F90, f77
AIX	IBM		F90	F90
LINUX		PGI	F90	F90
LINUX	INTEL			F90
OS X	APPLE	ABSOFT	F90	F90
OS X	APPLE	GNU	G77	G77

LBLRTM has previously been run on DEC alpha, Cray, MS-DOS, and HP platforms.

In addition, some users have ported the code to the Windows/DOS environment. However, AER does not officially support this implementation and recommend using UNIX or LINUX-based platforms.

3.2 Issues relating to unformatted files on UNIX and LINUX systems

Binary files are often not compatible between systems due to differences in the way the bytes are written to the files (big-endian versus little-endian). Note that the “byteswap” option available with most compilers will not work with most LBLRTM binary output files because of the mixing of real and integer data within records.

3.3 LNFL/LBLRTM Naming Convention

Specific information on the input/output files from LNFL and LBLRTM is located in their respective input files, `lnfl_instructions` and `lblrtm_instructions`, and the examples provided in the code tar files.

Most file names are given as “TAPE x ” where x is a one- or two-digit number. The name is case-sensitive, and is uppercase. Tape numbers may be same for LNFL and LBLRTM but do not represent identical files. For example, the primary LNFL input file is TAPE5, and the primary LBLRTM input file is TAPE5. However, they have neither the same input information nor the same formatting. The instruction manual for each code details the input file information.

3.4 LNFL/LBLRTM Input File (TAPE5) Format

The TAPE5 input files are read as formatted FORTRAN. As a consequence of the formatted read, any blank space will be read as “zero”. Thus, one may leave blanks for most of the parameters and within the code they will default to an acceptable value.

Real numbers format input as either “E” or “F” format, with the entire number within the range specified in the input instructions. Integers must be specified exactly in the integer format. For example, the spectral bandwidth (v_1 to v_2) in LBLRTM TAPE5 is input as 10 character real

numbers. This means that the value can be written anywhere within these 10 characters, as long as there is a decimal point (e.g. "---600.000" or "-600.000--", where "-" is a blank space).

Integers are read in with the "I" format. For example, the model atmosphere (iatm) in LBLRTM TAPE5 is input as "I5", so it must be "----2", and not "2----" as this will be read as 20000.

3.5 LBLRTM Output File Format

The general structure of the files involves the use of panels, which are blocks of output usually containing 2400 points. Each panel contains a header to describe the starting and ending points of the panel (v1 and v2), the spectral spacing of the points (dvp), and the number of points in the panel (npts). The panel header is followed by either one or two (see below) blocks of output, consisting of npts points.

TAPE12: Radiances and transmittances

(1) file header

(2,i)-panel header

(3,i) radiances

(4,i) transmittances

Lines 2-4 repeat for i=1,N times to cover the entire spectral region.

TAPE11: Filtered radiance or transmittance (also applies to any user-designated output file which contains radiances, transmittances, or optical depths, such as the "ODint" file)

(1) file header

(2,i)-panel header

(3,i) radiances or transmittances\

Lines 2-3 repeat for i=1,N times to cover the entire spectral region.

Note that a limited amount of spectral output information may also be put in the TAPE6 using the MPTS/NPTS options of TAPE5 record 1.2.

4 Instructions and Tips for Running LNFL

LNFL is used to generate a binary file (TAPE3) of all the line parameters required by LBLRTM.

4.1 Input files for LNFL

TAPE1: The line parameter database in ASCII format (also available on www.rtweb.aer.com).

TAPE5: LNFL input file.

4.2 Output files for LNFL

TAPE3: Binary LNFL output file containing the line parameters for LBLRTM.

TAPE6: Informational output file.

DRAFT
Page 5 of 12

TAPE7: Optional output file containing ASCII version of the parameters contained in TAPE3.

4.3 Sequence for running LNFL

- * Download latest LNFL tar code (containing the source code) and the latest line parameter database from rtweb.aer.com.
- * Compile LNFL using the makefiles found in the LNFL tar file. Note, one needs to compile in the directory above the makefile directory (i.e. `make -f makefile/makeInfl.xxxxx`)
- * Link the line parameter database to TAPE1 in the LNFL working directory.
- * Remove any TAPE2 or TAPE3 files from the LNFL working directory.
- * Edit necessary parameters in the TAPE5 input file. Note that the beginning and ending wavenumber (v_1 , v_2) in TAPE5 must be 25 cm^{-1} larger than the desired spectral range for the LBLRTM calculations.
- * Run the LNFL code.

5 Instructions and Tips for Compiling and Running LBLRTM

LBLRTM is used to generate line-by-line upwelling and downwelling transmittances and radiances.

5.1 Required input files for LBLRTM

TAPE3: Binary file containing line parameter information, generated by LNFL (see above). The TAPE3 file should include lines from at least 25 cm^{-1} on either end of the calculation region.

TAPE5: Input file required to run LBLRTM.

The spectral interval (v_1 , v_2) for any LBLRTM run must not exceed 2000 cm^{-1} (see instruction manual).

Other input files are required if you are using the solar source function, cross sections, surface emissivity, etc. See the LBLRTM instruction manual and provide example.

5.2 Layer numbering scheme

The LBLRTM convention is that layer 1 is at the highest pressure level (lowest altitude). The layer information for a given run may be found in TAPE6.

5.3 Output files for LBLRTM

TAPE6: Informational output file

TAPE11: Unformatted binary file containing filtered output, if requested in TAPE5.

TAPE12: Unformatted binary file containing transmittances/radiances.

ASCII file of unformatted binary files can be requested in the LBLRTM TAPE5 (see `pltbl` variable in Record 12).

Unformatted optical depth files can be requested in the LBLRTM using options specified in TAPE5.

5.4 Sequence for running LBLRTM

- * Download latest LBLRTM tar code (containing the source code) and the latest line parameter database from rtweb.aer.com.
- * Compile LBLRTM following makefiles in the LNFL tar file. Note, one needs to compile in the directory above the makefiles directory (i.e. `make -f makefiles/makelbl.xxxxx`)
- * Link the line parameter database (TAPE3 from LNFL) to LBLRTM working directory.
- * Edit any parameters necessary in the input file TAPE5.
- * Run the LBLRTM code.

6 General Questions

6.1 What is the difference between a line-by-line calculation and a band-model calculation?

Absorption/emission spectra are comprised of a complicated array of spectral lines. The HITRAN2000 Database (Version 11.0) contains over 1,080,000 spectral lines for 36 different molecules. In order to resolve these individual lines, a nominal spectral sampling rate of less than the mean line half width must be utilized. Such highly resolved radiative transfer calculations are called line-by-line (LBL) calculations. The computational time associated with calculating broadband fluxes from LBL calculations is formidable. A band model aims to simplify radiative transfer calculations by using approximations to represent the line-by-line characteristics of a particular spectral interval. Band models are appropriate for situations where the desired spectral resolution is much smaller than the Lorentz and Doppler widths of the spectral lines. Such approximations are also of use in general circulation models.

6.2 What are the standard units used in LBLRTM calculations?

Wavenumber: cm^{-1}

Radiance: $\text{W}/(\text{cm}^2 \text{ sr cm}^{-1})$

Brightness Temperature: K

Analytic Jacobians (dR/dx):

molecules: $[\text{W} / (\text{cm}^2 \text{ sr cm}^{-1})] / [\log(\text{volume mixing ratio})]$

temperature: $[\text{W} / (\text{cm}^2 \text{ sr cm}^{-1})] / [\text{K}]$

DRAFT

6.3 Radiance Derivatives (Jacobians)

The implementation of analytic Jacobians in LBLRTM was designed to require a minimal amount of setup on the part of the user while exploiting pre-existing LBLRTM calculation options. It is apparent from the equations for analytic derivatives that a number of different optical depth files are required: layer optical depth and total optical depth from the layer to the top and bottom of the atmosphere. These are created in a pre-processing run of LBLRTM using the IMRG=10 option. This option (modified slightly for the calculation of analytic Jacobians) will create, for each layer, files containing the total optical depth (ODint) and files containing the total optical depth from the layer to the top (ODtoupw) and bottom (ODtodnw) of the atmosphere (that is, the upwelling “upw” and downwelling “dnw” terms). As described in the specific user instructions, below, these files are created for a user-specified, fixed wavenumber grid for all layers using the “odint” and “dvset” options. Note that following LBLRTM convention, the layer 1 is that at the highest pressure level (lowest altitude).

Following this IMRG=10 run of LBLRTM, subsequent runs are done using the IMRG=40,41 options with IEMIT=3 to compute the single-species optical depths (necessary when computing the molecular derivatives) and assemble the analytic derivative files. If the user has requested the derivative for upwelling radiation, the code automatically makes the calculation of downwelling derivatives required for the upwelling derivatives. A single run of LBLRTM is required for each of the desired derivatives. The layer to level conversion is done after the layer derivative files are created, but only if level information was provided in the LBLRTM input file. Note that it is required that the input profile values be on the same grid as the specified model levels in order to maintain high accuracy when computing the layer to level conversion. In addition to monochromatic derivatives it is also possible to “scan” the derivative files (IMRG=42,43 options with IEMIT=3) to create files representative of a particular sensor response function, or simply to reduce the number of points in the output file for cases where high spectral resolution is not required. Examples of the TAPE5 format are given in Figure 1 and Figure 2.

LNFL/BLRTM
Frequently Asked Questions

```
-- test of layer ---
$ compute od
HI=1 F4=1 CN=1 AE=0 EM=0 SC=0 FI=0 PL=0 TS=0 AM=0 MG10 LA=0 OD=3 XS=0 0 0
950. 1050. 3.0E-03
1 5 7 1.000000U. S. STANDARD, H1= 0.00 H2= 10.00 ANG= 0.000 LEN= 0
431.9719 245.00 1 6.300 452.973 247.25 7.000 411.100 242.70
6.0912993E+20 3.2173082E+20 4.1773694E+16 2.8598304E+17 1.1273203E+17 1.5187077E+18 1.8678222E+23 7.0590631E+23
391.5240 240.45 1 7.700 372.071 238.15
4.0665826E+20 2.9720584E+20 4.3953746E+16 2.6418291E+17 1.0115719E+17 1.4020756E+18 1.5899987E+23 6.0089354E+23
354.2126 232.90 1 8.400 336.245 233.60
2.6413072E+20 2.7387547E+20 4.3173421E+16 2.4340233E+17 8.9662270E+16 1.2907807E+18 1.6646673E+23 6.2912967E+23
317.5832 231.04 1 9.200 298.875 228.42
1.5283365E+20 2.8673683E+20 6.7028694E+16 2.5453997E+17 8.8570798E+16 1.3490399E+18 1.6646673E+23 6.2912967E+23
281.8736 225.89 1 10.000 265.000 223.30
7.1713895E+19 2.6014855E+20 8.2274746E+16 2.3019499E+17 7.4799699E+16 1.2199868E+18 1.5103067E+23 5.7078877E+23
0
$ compute derivatives
HI=1 F4=1 CN=1 AE=0 EM=3 SC=0 FI=0 PL=0 TS=0 AM=0 MG41 LA=0 OD=3 XS=0 0 0
950. 1050. 3.0E-03 0.02
245.0 0.98
ODint_
ODtoupw_
ODtodnw_
1 5 7 1.000000U. S. STANDARD, H1= 0.00 H2= 10.00 ANG= 0.000 LEN= 0
431.9719 245.00 1 6.300 452.973 247.25 7.000 411.100 242.70
6.0912993E+20 3.2173082E+20 4.1773694E+16 2.8598304E+17 1.1273203E+17 1.5187077E+18 1.8678222E+23 7.0590631E+23
391.5240 240.45 1 7.700 372.071 238.15
4.0665826E+20 2.9720584E+20 4.3953746E+16 2.6418291E+17 1.0115719E+17 1.4020756E+18 1.5899987E+23 6.0089354E+23
354.2126 232.90 1 8.400 336.245 233.60
2.6413072E+20 2.7387547E+20 4.3173421E+16 2.4340233E+17 8.9662270E+16 1.2907807E+18 1.6646673E+23 6.2912967E+23
317.5832 231.04 1 9.200 298.875 228.42
1.5283365E+20 2.8673683E+20 6.7028694E+16 2.5453997E+17 8.8570798E+16 1.3490399E+18 1.6646673E+23 6.2912967E+23
281.8736 225.89 1 10.000 265.000 223.30
7.1713895E+19 2.6014855E+20 8.2274746E+16 2.3019499E+17 7.4799699E+16 1.2199868E+18 1.5103067E+23 5.7078877E+23
0
XXXX
--:-- TAPE5 11:28AM Mail (Fundamental)--L1--All-----
Minibuffer window is not active
```

Figure 1: Example TAPE5 format for layer calculation.

```
$ first create pre-stored od files (level input)
HI=1 F4=1 CN=1 AE=0 EM=0 SC=0 FI=0 PL=0 TS=0 AM=1 MG10 LA=0 OD=3 XS=0 00 00
950.000 1050. 3.7E-03
0 2 4 1 0 7 0 0 0 0.000 0.000 358.000
10.0000 8.0000 180.0000
8.000 8.700 9.500 10.000
4
INPUT FOR A-D Test
8.000 375.300 245.650 AA L AAAAAA
1.96130005e+02 3.58000000e+02 4.63050016e-02 3.19999993e-01 1.19360000e-01 1.69729996e+00 2.09000000e+05
8.700 325.700 237.850 AA L AAAAAA
9.96100006e+01 3.58000000e+02 4.45199988e-02 3.19570005e-01 1.10629998e-01 1.69350004e+00 2.09000000e+05
9.500 300.800 230.150 AA L AAAAAA
8.17360001e+01 3.58000000e+02 5.01900009e-02 3.18839997e-01 1.05370000e-01 1.68970001e+00 2.09000000e+05
10.000 274.700 228.750 AA L AAAAAA
4.67280006e+01 3.58000000e+02 5.69100012e-02 3.17799985e-01 9.93639976e-02 1.68470001e+00 2.09000000e+05
$ second, compute derivatives
HI=1 F4=1 CN=1 AE=0 EM=3 SC=0 FI=0 PL=0 TS=0 AM=1 MG41 LA=0 OD=3 XS=0 0 0
950. 1050. 3.7E-03 0.02
250.0 0.98
ODint_
ODtoupw_
ODtodnw_
0 2 4 1 0 7 0 0 0 0.000 0.000 358.000
10.0000 8.0000 180.0000
8.000 8.700 9.500 10.000
4
INPUT FOR A-D Test
8.000 375.300 245.650 AA L AAAAAA
1.96130005e+02 3.58000000e+02 4.63050016e-02 3.19999993e-01 1.19360000e-01 1.69729996e+00 2.09000000e+05
8.700 325.700 237.850 AA L AAAAAA
9.96100006e+01 3.58000000e+02 4.45199988e-02 3.19570005e-01 1.10629998e-01 1.69350004e+00 2.09000000e+05
9.500 300.800 230.150 AA L AAAAAA
8.17360001e+01 3.58000000e+02 4.71900009e-02 3.18839997e-01 1.05370000e-01 1.68970001e+00 2.09000000e+05
10.000 274.700 228.750 AA L AAAAAA
4.67280006e+01 3.58000000e+02 5.69100012e-02 3.17799985e-01 9.93639976e-02 1.68470001e+00 2.09000000e+05
XXX
--:-- TAPE5<2> 11:36AM Mail (Fundamental)--L1--All-----
```

Figure 2: Example TAPE5 format for level calculation.

Upon completion of the IMRG=40-43 run, the Jacobian files exist in the “AJ/” subdirectory. These files are of the form RDderivDNW_xx_zzz and RDderivUPW_xx_zzz for the downwelling and upwelling Jacobians, respectively. The two digit value of “xx” signifies the parameter for which the derivative is calculated (00 = temperature, 1 = H₂O, etc., following the HITRAN molecule numbering convention), while “yyy” is the three digit layer number. If the input (TAPE5) atmosphere is specified on levels, the layer-to-level conversion is performed. The level files have the prefix “LEV_”. The layer files have the same format as TAPE12 files (i.e. a file header followed by a repeating two-panel structure of 2400 points; the first panel is the Jacobian and the second panel is the total transmission), while the level files contain only single panels. (Note that by convention, the scanned layer files for IMRG=42,43 will only have a single panel).

Within the code, the calculation of analytic derivatives is as follows. As mentioned above, the first run of the code (IMRG=10) is used to compute the total optical depth for each layer and the transmission to the top and bottom of the atmosphere (in LBLRTM nomenclature, transmission from each layer to H1 and H2). For the derivative run of the code, all molecules are zeroed (automatically) except for the geophysical parameter desired for the calculation (care is taken to ensure that the other amounts are properly included in the calculation of broadening gases) in order to compute the single-species optical depth required for the molecular Jacobian calculation. For each layer, the code loops over each panel to compute the layer derivative. For the case of upwelling derivatives, the code is first set (automatically) to compute the downwelling derivative. These files are then used in the subsequent upwelling calculation (along with information about surface emissivity, temperature, and reflectivity, as necessary).

6.4 Does LBLRTM include heavy molecule parameters (cross-sectional species)?

Heavy molecules (such as CCL₄, F11, and others listed in Table II of the lblrtm_instruction manual) can be included in LBLRTM calculations by setting the IXSECT input variable to 1 and adding Record 2.2 or Record 3.7 to the LBLRTM TAPE5. An additional file (FSCDXS) and directory (xs) are required for these calculations and can be obtained from the LBLRTM example tar file (available from rtweb.aer.com).

6.5 Format of external surface emissivity/reflectivity files

Sea surface spectral emissivity/reflectivity files are provided with the example (available from www.rtweb.aer.com). The files must have the file names of “EMISSION” and “REFLECTIVITY”. The format is as follows:

V1EMIS, V2EMIS, DVEMIS, NLIMEM
(3E10.3,5X,I5)
ZEMIS(1...N)
(E15.7)

DRAFT
Page 10 of 12

V1EMIS -> Initial emissivity/reflectivity frequency value (cm-1)
V2EMIS -> Final emissivity/reflectivity frequency value (cm-1)
DVEMIS -> Is the frequency increment (cm-1)
NLIMEM -> Number of spectral emissivity/reflectivity points in the file

*Note: It is assumed that the spectral emissivity/reflectivity points are equally spaced.

6.6 Absorption due to clouds/aerosols and LOWTRAN5 routines

Absorption due to clouds and aerosols can be computed in LBLRTM by setting the IAERSL flag in the input TAPE5 file (refer to instructions). This flag allows for LBLRTM to utilize the aerosol capabilities of LOWTRAN5.

6.7 Solar Radiance

Solar radiance calculations can be performed by utilizing LBLRTM input options such as IEMIT=2 and a particular solar source function file SOLAR.RAD. A SOLAR.RAD file can be generated with program extract_solar available on the AER RT web site and the Kurucz solar source function. The Kurucz solar source function has been used in AER's research in shortwave radiation and is based on theoretical radiative transfer calculations for the solar atmosphere. The solar source function is available at a high spectral resolution (i.e. for monochromatic calculations) and 1 cm⁻¹ resolution.

6.8 Line coupling

The line coupling parameters are added to the LBLRTM input TAPE3 by LNFL (refer to LNFL instruction manual).

Gas	Line Coupling Spectral Range
O2	0.0-1.0E-05
O2	1.666572 - 3.961085
CO2	612.196012 - 618.023765
CO2	667.386195 - 676.414878
CO2	714.584932 - 721.574672
CO2	735.944778 - 741.722273
CO2	791.452602 - 795.038363
CO2	1932.478947 - 1936.074343
CO2	2076.862561 - 2079.779298
CO2	2093.346577 - 2097.908961
CO2	2128.359397 - 2129.752135

6.9 What is the appropriate reference for LBLRTM calculations in journal articles and presentations?

Clough SA, Shephard MW, Mlawer EJ, Delamere JS, Iacono MJ, Cady-Pereira K, Boukabara S, Brown PD. Atmospheric radiative transfer modeling: a summary of the AER codes • SHORT COMMUNICATION • J Quant. Spectrosc. and Radiat Transfer, In Press, Corrected Proof, Available online 28 July 2004.

Also, please refer to rtweb.aer.com for the complete list of references.

6.10 How do you calculate fluxes?

Source code and instructions available: http://rtweb.aer.com/radsum_frame.html

DRAFT