**Design for MT-CKD H2O for HITRAN and LBLRTM**

## Flow Chart

Diagram

Description automatically generated

## Components

## Cntnm\_internal: FORTRAN90

This is the internal version of the continuum code, which will allow Eli to continue his continuum development work as he is accustomed to, i.e., modifying the DATA statements and the coefficient calculations. The code outputs the water continuum coefficients in a modern and portable format for use by the mt\_ck\_h2o routine.

**Output:** absco-ref\_wv-mt-ckd.nc

Below is a listing of the absco-ref\_wv-mt-ckd.nc contents:

netcdf absco-ref\_wv-mt-ckd {

dimensions:

wavenumbers = 2001 ;

variables:

double wavenumbers(wavenumbers) ;

wavenumbers:units = "cm-1" ;

wavenumbers:description = "Spectral domain of water vapor continuum" ;

double self\_absco\_ref(wavenumbers) ;

self\_absco\_ref:units = "cm\*\*2/molecule cm-1" ;

self\_absco\_ref:description = "Water vapor self continuum absorption coefficients" ;

double for\_absco\_ref(wavenumbers) ;

for\_absco\_ref:units = "cm\*\*2/molecule cm-1" ;

for\_absco\_ref:description = "Water vapor foreign continuum absorption coefficients" ;

double self\_texp(wavenumbers) ;

self\_texp:units = "dimensionless" ;

self\_texp:description = "Temperature exponent for water vapor self continuum" ;

double ref\_press ;

ref\_press:units = "mbar" ;

ref\_press:description = "Reference pressure" ;

double ref\_temp ;

ref\_temp:units = "K" ;

ref\_temp:description = "Reference temperature" ;

double ref\_h2o\_vmr ;

ref\_h2o\_vmr:units = "vmr" ;

ref\_h2o\_vmr:description = "Reference H2O Mixing Ratio" ;

// global attributes:

:title = " The MT\_CKD Water Vapor Continuum - v4.0 " ;

:copyright = "Copyright �, Atmospheric and Environmental Research, Inc., 2022 All rights reserved. This source code was developed as part of the LBLRTM software and is designed for scientific and research purposes. Atmospheric and Environmental Research Inc. (AER) grants USER the right to download, install, use and copy this software for scientific and research purposes only. This software may be redistributed as long as this copyright notice is reproduced on any copy made and appropriate acknowledgment is given to AER. This software or any modified version of this software may not be incorporated into proprietary software or commercial software offered for sale without the express written consent of AER. This software is provided as is without any express or implied warranties." ;

:contact = " Address questions to: aer\_contnm@aer.com " ;

:reference = " General reference: Mlawer et al. (2012), doi:10.1098/rsta.2011.0295 " ;

:history = "MT\_CKD\_4.0: water vapor continuum data is now stored in a netCDF file and the code is in a separate module.For previous versions see (http://github.com/AER-RC/MT\_CKD). " ;

## mt\_ckd\_h2o\_module: FORTRAN90

This module contains the mt\_ckd\_h2o\_absco subroutine, which reads in the absco-ref\_wv-mt-ckd netCDF file and calculates the water vapor continuum absorption coefficients for the requested pressure, temperature, and spectral range. The mt\_ckd\_h2o\_absco subroutine can be called from a simple driver (see section d) or from the LBLRTM CONTNM subroutine: it replaces the lines of code, including DATA statements and spectral interpolation, that are currently required in the CONTNM routine for the water vapor continuum absorption calculation. The output is provided in the sh2o and fh2oarrays, which must be declared in the calling program. The module also contains three short private routines adapted from LBLRTM: myradfn, myxint and pre\_xint.

mt\_ckd\_h2o\_absco uses the get\_data routine in the read\_data module to read in absco-ref-wv-mt-ckd.nc file. The module will be provided to SAO, along with the read\_data module, the absco-ref\_wv-mt-ckd.nc file and a simple FORTRAN driver to run the module.

**mt\_ckd\_h2o\_absco**

**Definition:** subroutine mt\_ckd\_h2o( p\_atm,t\_atm ,h2o\_frac,wv1,wv2,dwv,self\_absco, for\_absco, radflag)

**Inputs:**

p\_atm - atmospheric pressure for the calculation of continuum coefficients (mbar)

t\_atm - atmospheric temperature for the calculation of continuum coefficients (K)

h2o\_frac - fraction of the total number of molecules that are water vapor

wv1abs - initial wavenumber for which continuum coefficients will be computed (cm-1)

wv2abs - final wavenumber for which continuum coefficients will be computed (cm-1)

dvabs - wavenumber spacing for the continuum coefficient calculation (cm-1)

radflag - (optional) if true, multiply by radiation term (default); if false, do not

**Input/Output:**

self\_absco - computed water vapor self continuum absorption coefficients (cm2/molecules or 1/(cm-1 molecules/cm2)

for\_absco - computed water vapor foreign continuum absorption coefficients (cm2/molecules or 1/(cm-1 molecules/cm2)

**myradfn:** calculates the radiation term for a specific temperature and an array of frequencies. Note that the radfn function in LBLRTM calculates this term for a single frequency

**Definition:** integer function myradfn (vi,xkt,nvi,rad)

**Inputs:**

v1: array of frequencies (cm-1)

xkt: ratio of layer temperature to radcn2 (cm-1)

nvi: number of frequencies in v1

**Outputs:**

rad: array of radiation terms (cm-1)

**pre\_xint:** finds the starting and ending indices to use in the interpolation to the requested

grid

**Definition:** subroutine pre\_xint(v1ss,v2ss,v1abs,dvabs,nptabs,ist,lst)

**Inputs:**

v1ss: first frequency of coefficient grid (cm-1)

v2ss: last frequency of coefficient grid (cm-1)

v1abs: first frequency of output grid (cm-1)

v2abs: last frequency of output grid (cm-1)

dvabs: resolution of output grid (cm-1)

nptabs: number of points in output grid

**Outputs:**

ist: index of first point to interpolate to in output grid

lst: index of last point to interpolate to in output grid

**myxint:** interpolates to output grid and adds to existing absorption/optical depth

**Definition:** subroutine myxint(v1a,v2a,dva,a,afact,vft,dvr3,r3,n1r3,n2r3)

**Inputs:**

v1a: first frequency of coefficient grid (cm-1)

v2a: last frequency of coefficient grid (cm-1)

dva: resolution of coefficient grid (cm-1)

a: array of calculated absorption (cm2/molec) or optical depth

afact: 1.0

vft: starting frequency of output grid (cm-1)

dvr3: resolution of output grid (cm-1)

n1r3: index of first point to interpolate to in output grid

n2r3: index of last point to interpolate to in output grid

**Input/Output**

**r**3: array of interpolated and summed absorption (molec/cm2) or optical depth

## read\_ module: FORTRAN90

This module defines a data type (data2read) to store the contents of absco-ref\_wv-mt-ckd.nc, reads in the contents of this file with the get\_data routine and returns them to the calling routine in the defined datatype.

**Input:** absco-ref\_wv-mt-ckd.nc

**Output:** dat: user defined datatype data2read containing all the data in absco-ref\_wv-mt-ckd.nc:

type data2read

real(kind=8), allocatable, dimension(:) :: wavenumber

real(kind=8), allocatable, dimension(:) :: for\_absco\_ref

real(kind=8), allocatable, dimension(:) :: self\_absco\_ref

real(kind=8), allocatable, dimension(:) :: self\_texp

* 1. drive\_mt\_ckd\_h20.f90: FORTRAN

drive\_mt\_ckd\_h2o is a simple FORTRAN driver for mt\_ckd\_h2o. It reads in the required inputs for absco-ref\_mt-ckd-h2o from a NAMELIST file and outputs the spectral grid and the self and foreign coefficients in a netCDF file.

Below is a sample namelist file:

&mt\_ckd\_input

p\_atm=1013.

t\_atm=300.

h2o\_frac= 0.00990098

wv1=497.

wv2=603.

dwv=1.

/

The code is compiled with the following command in the build directory (see section **3.**)

make -f make\_mt\_ckd\_h2o linuxGNUdbl

where make\_mt\_ckd\_h2o is the Makefile and linuxGNUdbl indicates the user has requested the gfortran compiler with double precision.

This command generates the mt\_ckd\_h2o\_v1.0\_linux\_gnu\_dbl executable, which is run as indicated below:

mt\_ckd\_h2o\_v1.0\_linux\_gnu\_dbl < mt\_ckd.config

where mt\_ckd.config is the namelist file.

The output is stored in mt\_ckd\_h2o\_output.nc:

netcdf mt\_ckd\_h2o\_output {

dimensions:

nwvn = 107 ;

variables:

double wavenumbers(nwvn) ;

wavenumbers:units = "cm-1" ;

wavenumbers:description = "Wavenumbers\f" ;

double self\_absorption(nwvn) ;

self\_absorption:units = "cm\*\*2/molecule)" ;

self\_absorption:description = "Water vapor continuum self absorption coefficients" ;

double frgn\_absorption(nwvn) ;

frgn\_absorption:units = "cm\*\*2/molecule)" ;

frgn\_absorption:description = "Water vapor foreign continuum absorption coefficients" ;

## **Directory structure**

**mt\_ckd\_h2o:**

absco-ref\_wv-mt-ckd.nc build/ mt\_ckd.config mt\_ckd\_h2o\_output.nc src/

**mt\_ckd\_h2o/build**:

addlibs.inc make\_mt\_ckd\_h2o\* mt\_ckd\_h2o\_v1.0\_linux\_gnu\_dbl.obj/ read\_file.mod

makefile.common\* mt\_ckd\_h2o.mod phys\_consts.mod

**mt\_ckd\_h2o/src:**

drive\_mt\_ckd\_h2o.f90 mt\_ckd\_h2o\_module.f90 phys\_consts.f90 read\_module.f90

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