Technical note on:

Installation and code description of the line-selection tool for microwindow databases: linselmw

January 3, 2000

Draft Version

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1. Necessary files

- Files for code-compilation:

  - `linselmw_1.0.f` (source code)
  - `linselmw_para.inc` (parameter include file)

- File with fixed name that must be present in the actual directory from where the program is called:

  - `NESR.tab` (table with NESR values for MIPAS)

- File from which the program reads (standard input)

  - control input file for linselmw

- Files to run the program for which the names and directories are given in the control input file:

  - File for pressure, temperature and gas vmr profiles to be considered for the target gases
  - File for pressure, temperature and gas vmr profiles to be considered for the interfering gases
  - HITRAN file with spectroscopic data
  - Microwindow database files

2. Compiling the source code

Use any standard fortran 77 compiler to compile the source code `linselmw_1.0.f.` Make sure that the parameter include file `linselmw_para.inc` is present in the compilation directory.

```
f77 -o linselmw linselmw_1.0.f
```

3. Running the program

Make sure that the file `NESR.tab` is in the actual directory. Run the code by typing

`linselmw <` control-input-file-name

4. Description of the input files

4.1 NESR.tab

This file must be present in the directory where the program is called. It contains the (unapodized) NESR values of MIPAS which are use for the line-selection criteria. The format is:

```
6.800000e+02        6.974779e-08
6.900000e+02        6.974779e-08
7.000000e+02        5.787196e-08
7.100000e+02        4.853187e-08
7.200000e+02        4.269490e-08
...       ...
```

Where the first row contains the wavenumbers [cm^{-1}] and the second row the NESR [$W/(cm^2 sr\ cm^{-1})$]. The number of NESR grid points is MXNESR=175, a parameter defined in `linselmw_para.inc`.

4.2 control-input-file

The control input file of the program and is read from standard input. The line(s) after a line which begins with $ contain the input which is read by the code. In the following an example of the file is given.

File for pressure, temperature and gas vmr profiles to be considered for the target gases

```
$1
/home/michael/Projects/CCN5/Linesel/input/std.prf
```

File for pressure, temperature and gas vmr profiles to be considered for the interfering gases

```
$2
/home/michael/Projects/CCN5/Linsel/input/max.prf
```

HITRAN file name

```
$3
/home/michael/Projects/CCN5/Linsel/input/hitran96_o3new+
```

Number of microwindow databases for which lines should be selected

```
$4
 3
```

Hitran number of targets for each microwindow database

(PT=2, O3=3, H2O=1, N2O=4, CH4=6, NO2=10, HNO3=12)

```
$5
 2
 1
 3
```

File names for each microwindow database

```
$6
/home/michael/Projects/CCN5/MW_oxf/MW_PT__103.DAT
/home/michael/Projects/CCN5/MW_oxf/MW_H2O_003.DAT
/home/michael/Projects/CCN5/MW_oxf/MW_O3__003.DAT
```

Directory names for output of microwindow linedata files
(one per microwindow database)

```
$7
/home/michael/Projects/CCN5/Linsel/output/PT__103/
/home/michael/Projects/CCN5/Linsel/output/H2O_003/
/home/michael/Projects/CCN5/Linsel/output/O3__003/
```

4.3 $1 and $2 of linselmw.inp

These are the files for pressure, temperature and gas vmr profiles to be considered for the target and interfering gases. Again the program reads input after the $ signs.

Number of atmospheric levels

```
$
   121
```

Level altitudes [km]

```
$
  0.000E+00  1.000E+00  2.000E+00  3.000E+00  4.000E+00
  ...
```

Level pressures [hPa]

```
$
  1.010E+03  8.990E+02  7.950E+02  7.010E+02  6.170E+02
  ...
```

Level temperatures [K]

```
$
  2.882E+02  2.817E+02  2.752E+02  2.687E+02  2.622E+02
  ...
```

Number of gas profiles given below

```
$
  35
```

The gas profiles (all HITRAN molecules in ascending order) [ppmv]
(in the first line after the $ there is the HITRAN molecule number, in the following lines the related profile)

```
$
   1
  7.750E+03  6.070E+03  4.630E+03  3.180E+03  2.160E+03
  ...

$
   2
  3.550E+02  3.550E+02  3.550E+02  3.550E+02  3.550E+02
  ...

.
.
.

$
 35
6.000E-06  5.000E-06  4.400E-06  3.800E-06  3.100E-06
  ...
```

4.4 $3 of linselmw.inp

A standard HITRAN file with the spectroscopic data.

4.5 $6 of linselmw.inp

Standard microwindow database files.

5. Description of the output files

The output files containing the spectroscopic data for the selected lines are written into the directories as specified under `$7` of the control input file. For each microwindow one file is created. The file names are `SP_`mw-name`.DAT` where mw-name is identical with the microwindow names as given in the microwindow databases (format: *ggggnnnn* with *gggg* = main gas, trailing blanks filled with _'s; *nnnn* = identifier with leading zeros).

The format of the files is similar to the HITRAN96 format. It is compatible with the format of the 'Spectroscopic Data Input Files' as described in the 'Interface Control Document' (PO-IF-DOG-GS-0002, issue 1C, date 29.10.99). Each file contains three header lines and a number of lines providing the spectroscopic data for each transition. The format is listed in the table below.

1st record	
A27	Date and time of creation
2nd record	
A	Comment line starting with '#'
3rd record	
A8, 5x	Spectroscopic data base used for the generation
A8, 5x	Name of the microwindow
A24, 5x	Data and time of generation
I5	Number of spectroscopic transitions (number of records following in the file)
Next records: one record for each transition (record length 100) (same format as HITRAN96, but the transition probability is replaced by the two altitdes within which the lines should be considered, and an integer flag for the line wing treatment)	
I2	HITRAN molecule number
I1	Isotope number
F12.6	Wavenumber of transition [cm^{-1}]
1PE10.3	Intensity [cm-1/(molec × cm^{-2})] @ 296 K
F4.1	Lowest tangent altitdue the transition has to be considered [km]
F4.1	Highest tangent altitude the transition has to be considered [km]
I2	Flag for the line wing treatment =1 full treatment =0 interpolation possible
F5.4	Air-broadened halfwidth [cm^{-1}] @ 296 K
F5.4	Self-broadened halfwidth [cm^{-1}] @ 296 K
F10.4	Lower state energy [cm^{-1}]
F4.2	Coefficient of temperature dependence of air-broadened half-width
F8.5	Pressure shift [cm^{-1}]
I3	Upper state global quanta index
I3	Lower state global quanta index
A9	Upper state local quanta
A9	Lower state local quanta
I1	Accuracy index for wavenumber reference
I1	Accuracy index for intensity reference
I1	Accuracy index for halfwidth reference
I2	Lookup index for wavenumber
I2	Lookup index for intensity
I2	Lookup index for halfwidth

6. Description of the code

6.1 Loops, subroutine calls and description of the main program

* read the main control input file
 => `read_input`

* read file with nesr-values
 => `read_nesr`

* calculate Curtis-Godson values and partial columns (2-layer model) for
 the interfering species
 => `meanlayer`

* calculate Curtis-Godson values and partial columns (2-layer model) for
 the target species
 => `meanlayer`

BEGIN LOOP ON TARGET GASES

    * read microwindow database
     => `readtr`

    BEGIN LOOP ON MICROWINDOWS

        * read HITRAN database
         => `readhit`

        * calculate thresholds

        BEGIN LOOP ON TANGENT ALTITUDES

            ----
          * start line selection of lines outside microwindow:

            BEGIN LOOP ON LINES OUTSIDE MICROWINDOW

                * calculate line parameters
                 => `STRENGTH`

                * setting flag for the line wing tratment

* calculation of absorption coefficients
  => PLORENTZ

END LOOP ON LINES OUTSIDE MICROWINDOW

* calculation of radiances (2-layer model) at
  microwindow boundaries
  => RAD2

* sorting lines according to contribution to absorption
  coefficient and frequency variation of line shape
  => SORTAM1

* recalculate threshold if calculated radiances at mw
  boundaries are small

* reject lines with smallest contributions (as sorted before)
  until threshold is exceeded by radiances of rejected lines

* setting altitude region of lines

* end line selection of lines outside microwindow
  ---
* begin line selection of lines inside microwindow

* calculate line parameters
  => STRENGTH

BEGIN ITERATION LOOP FOR LINE SELECTION

BEGIN LOOP ON LINES i IN MICROWINDOW

* calculate contributions from lines outside mw
  to absorption coefficient at line center (i)

* initialize all lines to be neglected in first
  iteration

* calculate absorption coefficient at line
  center (i) under consideration of all neglected
  lines
  => VOIGT

* calculate radiance at linecenter (i)
  => RAD2

* setting up grid around line (i) for convolution
  with AILS (triangular apodization)

END LOOP ON LINES i IN MICROWINDOW

BEGIN LOOP ON LINES i IN MICROWINDOW

* calculation of convoluted radiance at line center (i) under consideration of all neglected lines (in the first iteration this is equal to radiances including all lines RMAX)

* if convoluted radiance is higher than threshold:
  - search for line j contributing most to radiance
  - if j = i: sort line i in list of considered lines
  - if more than 10 iterations: sort line i in list of considered lines

END LOOP ON LINES i IN MICROWINDOW

* if convoluted radiances of rejected lines at any line centers is lower threshold than leave iteration loop

END ITERATION LOOP FOR LINE SELECTION

END LOOP ON TANGENT ALTITUDES

* write line database

END LOOP ON MICROWINDOWS

END LOOP ON TARGET GASES

6.2 Description of main subroutines

6.2.1 subroutine meanlayer

Description
Calculate Curtis-Godson values and partial columns (2-layer model) for a set of pressure, temperature and trace gases vmr profiles.

Input/output variables

`Ptvmrfil`	File name of pressure, temperature and vmr profiles	In
`Nth`	Number of tangent heights	In
`Th`	Tangent heights	In
`Tgh`	Temperature at tangent heights	Out
`Pgh`	Pressure at tangent heights	Out
`th0`	Curtis-Godson temperature for total path	Out
`th1`	Curtis-Godson temperature for large path	Out

th2	Curtis-Godson temperature for small path	Out
tm0	Partial column for total path	Out
tm1	Partial column for large path	Out
tm2	Partial column for small path	Out
tp0	Curtis-Godson pressure for total path	Out
tp1	Curtis-Godson pressure for large path	Out
tp2	Curtis-Godson pressure for small path	Out

Sequence
- read pt-vmr –file
- calculate tangent height values of p and T
- calculate total columns
- calculate way for 96% of column
- calculate lower path (96%)
- calculate higher path (4%)

6.2.2 subroutine read_input

Description
Read the main control input file

Input/output variables

infil	Control input filename	In
ptvmrfil_tar	File name for target profiles	Out
ptvmrfil_itf	File name for interfering gas profiles	Out
hitfil	Hitran file name	Out
ntar	Number of microwindow databases for which lines should be selected	Out
mwfil	File names of microwindow databases	Out
spcdir	Directory names for output of microwindow linedata files	Out
ihittar	Hitran number of targets for each microwindow database (PT=2, O3=3, H2O=1, N2O=4, CH4=6, NO2=10, HNO3=12)	Out

Sequence
- read main control input file

6.2.3 subroutine readtr

Description
Read microwindow database

Input/output variables

ihittar	Hitran number of targets for each microwindow database (PT=2, O3=3, H2O=1, N2O=4, CH4=6,	In

	NO2=10, HNO3=12)	
mwfil	File name of microwindow database	In
nth	Number of tangent heights	In
th	Tangent heights	In
nmwmx	Number of microwindows	Out
mwname	Microwindow names	Out
vmin	Minimum wavenumber of each microwindow	Out
vmax	Maximum wavenumber of each microwindow	Out
ihmin	Lowest tangent altitude of each microwindow	Out
ihmax	Highest tangent altitude of each microwindow	Out
maxgas_mw	Number of gases per microwindow	Out
iglist_mw	Gaslist per microwindow	Out

Sequence
- read microwindow database
- order gaslist per microwindow so that target is first
- check if target gas is same as in input file (if not: use first gas in list as target gas)

6.2.4 subroutine readhit

Description
Read HITRAN database

Input/output variables

hitfil	HITRAN filename	In
na1	number of lines in [vmin-vdelta,vmin]	Out
na2	number of lines in[vmin-vdelta,vmin]and[vmax,vmax+vdelta]	Out
nti	number of target lines inside microwindow	Out
nsi	number of lines inside microwindow	Out
vmin	Minimum wavenumber of microwindow	In
vmax	Maximum wavenumber of microwindow	In
maxgas	Number of gases in microwindow	In
ig	Hitran molecule number for each line	Out
x	Wavenumber for each line	Out
s	Line strength for each line	Out
e	Lower state energy for each line	Out
a	Air-broadened halfwidth for each line	Out
tf	Coefficient of temperature dependence of air-broadened half-width for each line	Out
iglist	Gaslist	In
ic	Pointer to line numbering	Out
Igas	Hitran molecule number for each line	Out
Iso	Isotope number for each line	Out
Wnum	Wavenumber for each line	Out
Stren	Line strength for each line	Out
Trans	Transition probability for each line	Out

Abcoef	Coefficient of temperature dependence of air-broadened half-width for each line	Out
Abroad	Air-broadened halfwidth for each line	Out
Sbroad	Self-broadened halfwidth for each line	Out
En	Lower state energy for each line	Out
Y	Pressure shift for each line	Out
iv1	Upper state global quanta index	Out
iv2	Lower state global quanta index	Out
Q	Upper and lower state local quanta	Out
Ier	Accuracy indices	Out
Iref	Lookup reference indices	Out

Sequence
- read HITRAN database for actual microwindow

6.2.5 subroutine read_nesr

Description
Read mipas NESR table.

Input/output variables

nesrfil	Filename of NESR table (given in linselmw_para.inc)	In
mxnesr	Number of NESR values (given in linselmw_para.inc)	In
rfil	NESR wavenumbers	Out
fnesr	NESR values	Out

Sequence
- read NESR table