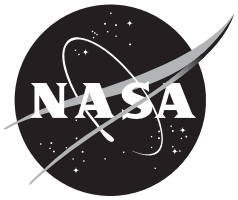

NEQAIRv14.0 Release Notes
Nonequilibrium and Equilibrium Radiative Transport Spectra Program

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1 Acknowledgements and NEQAIR Version History

The current version of [1]NEQAIR has been based upon[2] the work of many others across approximately 22 release versions of the code. A brief version of history of the code is shown in Table 1.

Table 1. Previous Authors of NEQAIR and Version History

Version	Year	Main Developers
HF730	1970s	Whiting, Arnold, Lyle
NEQAIR85	1985-1996	Chul Park
NEQAIR96	1996-1999	Whiting, Liu, et al
NEQAIR99x	1999-2007	Prabhu, Liu
NEQAIR2008	2008	David Saunders
NEQAIR2009v1-v8	2009-2012	Palmer, Cruden
NEQAIRv13.1-v13.2	2013	Cruden, Brandis
NEQAIRv14.0	2014 -	Cruden, Brandis

2 Introduction

NEQAIR v14.0 is the first parallelized version of NEQAIR. Starting from the last version of the code that went through the internal software release process at NASA Ames (NEQAIR 2008), there have been significant updates to the physics in the code and the computational efficiency. NEQAIR v14.0 supersedes NEQAIR v13.2, v13.1 and the suite of NEQAIR2009 versions. These updates have predominantly been performed by Brett Cruden and Aaron Brandis from ERC Inc at NASA Ames Research Center in 2013 and 2014.

A new naming convention is being adopted with this current release. The current and future versions of the code will be named NEQAIR vY.X. The Y will refer to a major release increment. Minor revisions and update releases will involve incrementing X. This is to keep NEQAIR more in line with common software release practices.

NEQAIR v14.0 is a standalone software tool for line-by-line spectral computation of radiative intensities and/or radiative heat flux, with one-dimensional transport of radiation. In order to accomplish this, NEQAIR v14.0, as in previous versions, requires the specification of distances (in cm), temperatures (in K) and number densities (in parts/cc) of constituent species along lines of sight. Therefore, it is assumed that flow quantities have been extracted from flow fields computed using other tools, such as CFD codes like DPLR (Wright, White, & Mangini, 2009) or LAURA (Mazaheri, Gnoffo, Johnston, & Kleb, 2010), and that lines of sight have been constructed and written out in the format required by NEQAIR v14.0.

There are two principal modes for running NEQAIR v14.0. In the first mode NEQAIR v14.0 is used as a tool for creating synthetic spectra of any desired resolution (including convolution with a specified instrument/slit function). The first mode is typically exercised in simulating/interpreting spectroscopic measurements of different sources (e.g. shock tube data, plasma torches, etc.). In the second mode, NEQAIR v14.0 is used as a radiative heat flux prediction tool for flight projects. Correspondingly, NEQAIR has also been used to simulate the radiance measured on previous flight missions.

This report summarizes the database updates, corrections that have been made to the code, changes to input files, parallelization, the current usage recommendations, including test cases, and an indication of the performance enhancements achieved.

3 Database Status

NEQAIR v13.2 and v14.0, use the atomic line data from v5.0.0 of the Atomic Spectroscopy Database (ASD, developed and supported by NIST - http://physics.nist.gov/PhysRefData/ASD/index.html) (Kramida, Ralchenko, & Reader, 2012). NEQAIR2009 versions had used v3.1 of the NIST database. Several updates relevant to NEQAIR occurred in NIST database v4.0.0, in particular for C and N. Atomic species that are currently present in the NEQAIR database include: N, O, C, H, He, Ar. Furthermore, all atomic (and molecular) lines are broadened according to Doppler, natural, Stark, van der Waals, and Resonance broadening mechanisms.

NEQAIR computes rotational lines in a diatomic molecular band system using Franck-Condon and Honl-London factors. The electronically excited diatomic band systems in the NEQAIR database include:

- N_2 (1^+), (2^+), (Birge-Hopfield I), (Birge-Hopfield II), (Carroll-Yoshino), (Worley), (Lyman-Birge-Hopfield)
- N_2^+ (1^-)
- O_2 (Schumann-Runge)
- NO (β), (γ), (δ), (ε), (β'), (γ')
- CO (4^+)
- CN (violet), (red)
- C_2 (Swan)
- OH (A-X)
- H_2 (B-X), (C-X), (B'-X)

Diatomic band system parameters come from various source including Gilmore et al. (Gilmore, Laher, & Espy, 1992), Laux, C. (Laux, 1993) and Hyun (Hyun, 2009).

The following vibrationally excited (IR) band systems are included in NEQAIR: NO, CN, CO, OH, NH, CH, and CO_2. The CO_2 model in NEQAIR is a reduction of the Carbon Dioxide Spectral Databank (CDSD) (Tashkun & Perevalov, 2011) covering the spectral region between 1600 and 10600 nm and contains 2.8 million individual lines plus a "pseudo-continuum," which parameterizes the effect of an additional 627 million weaker lines. For all other infra-red transitions, NEQAIR computes the molecular infrared transition probabilities using polynomial curve fits for dipole moments.

NEQAIR computes bound-free continuum radiation between ionized atomic species and electrons using data from TOPBase (Cunto, Mendoza, Ochsenbein, & Zeippen, 1993). NEQAIR also computes free-free continuum radiation using hydrogenic absorption coefficients with non-hydrogenic corrections according to the method of Peach (Peach, 1970). At present, free-free data only exists in NEQAIR databases for N, O, and C.

4 Summary of Updates/Bug Fixes Since NEQAIR2008v1

The following is a summary of some of the updates to the code, that bridge between the previously reported version of NEQAIR (2008), and the present version of the code:

- **NEQAIR2009v1:** reworking of NEQAIR2008 with a focus on code efficiency – approximately 10x faster than 2008.
- **NEQAIR2009v3:** miscellaneous clean up of the code, focus on use of modules, grid type added to input file.

- **NEQAIR2009v4:** a bug where the emission and absorption wasn't zeroed out if more than one region was being considered was fixed. Transport subroutine was streamlined.
- **NEQAIR2009v5:** molecular data no longer written to temporary files, but rather is stored in a common memory module. Scan feature restored using linear or Voigt slit function. Subroutines no longer needed were removed. Reduced number of required input files. Output written to data files instead of standard out. Improved commenting in the code.
- **NEQAIR2009v7a:** EAST slit functions added. Scan function now rigorously conserves energy, which was not the case before.
- **NEQAIR2009v7b:** The electronic level populations for molecular species are now computed in a single location. Previously, that code was spread and duplicated in several places throughout the code.
    - The molecular QSS routines now compute ratios of QSS to Boltzmann electronic level populations and make use of the Saha equation. This change was implemented to alleviate physically unrealistic results obtained when T_e is treated inconsistently between the CFD code and NEQAIR. (Generally, it is known that, for a two temperature radiation model, it is physically more meaningful to assign $T_e = T_v$, but the DPLR code typically uses $T_e = T_t$.)
- **NEQAIR2009v7c:** Sum of density of all states must equal total density (not necessarily true in previous versions). Time derivative of ground state unconstrained (this underlying QSS assumption was absent in v7B). More levels added to NO for QSS. Degeneracy error fixed for homonuclear molecules. Some other small bug fixes, removal of duplicate code and efficiency improvements.
- **NEQAIR2009v8:** Initial implementation of the CO_2 IR CDSD database.
- **NEQAIRv13.1:** Restructuring of 2009v8, variables and subroutines were updated to more intuitive names.

5 Summary of Recent Updates to NEQAIR (v13.2, v14.0)

- The mechanics of the QSS calculation have been substantially updated.
- QSS is now available for CO 4th Positive, CN Violet and therefore can be used for Mars, Titan and Venus entries (provided that the electron mole fraction is greater than 2.5E-5 in v13.2, this constraint has been lifted for v14.0).
- QSS updated for O_2 Schumann Runge.
- Mid-wave IR for CO_2 from CDSD database is extended over the full range.
- TOPBase data now used for continuum radiation. The bound-free database is substantially larger and took a long time to compute in v13.2. In v14.0 the looping structured was changed so that the overall computational time would not be substantially longer than in v13.1. The TOPBase cross sections have been shown to have improved agreement with EAST for Air conditions. These results have been shown in recent publications by Brandis et al. (Brandis, Wray, Liu, Schwenke, Huo, & Johnston, 2013) (Brandis A. , Johnston, Cruden, Prabhu, & Bose, 2012).
- Atomic line list updated to NIST 5.0. The NIST database is the standard used in the community and the current version has included new lines as compared to the previously employed line list. The update has provided minimal difference to total heat flux from N or O, but maybe have more impact with C containing atmospheres, as there are substantially more lines now.
- The CO 4th Positive database has been updated to that of da Silva as opposed to Rodio. Results showing that the da Silva database shows the best agreement with EAST is shown in (Brandis A. , et al., 2013).
- More robust generation of EHL Files (files used for molecular radiation calculations) in v13.2, and elimination of the files entirely in v14.0,
- Pre-dissociation rates added for O_2 and NO.

- Radiance as a function of distance behind the shock now output as LOS.out.
- Internal indexing of species simplified, as a consequence, a bug in the linewidth calculation was found and corrected.
- Scan process made more robust.
- NEQAIR now identifies and matches states assigned in the atomic Lines/Levels list, QSS (non-Boltzmann) calculation and TOP Base. These latter two use composite states. By matching these against the NIST level list, more accurate energies can be assigned to the composite states, giving more accurate overall calculations. An option to write out the level matching results (to LevelMatch.dat) is available by adding an X to the appropriate line in LEVELS_ATOMS.dat
- (v14.0) More accurate tangent slab/spherical cap approximation. Previous versions used an empirically weighted integral over angle, which under-predicted the true tangent slab solution by 1-2%, while v14.0 employs an adaptive integration routine which accurately converges the integration over angle to better than 1%.
- (v14.0) Parallel evaluation of different line of sight points. While v14.0 may be compiled in serial mode, the parallel evaluation is significantly faster, as will be discussed below.
- (v14.0) Added option to use Saha distribution of atomic excited states. Metastable states would still use a Boltzmann distribution
- (v14.0) Changed the controlling temperatures for reverse reaction rate/equilibration in QSS. This generally gives more stable solutions by making the QSS calculation more consistent with the rates used in CFD.
- (v14.0) Generally more efficient internal memory management.
- (v14.0) Removed upper bound constraint on size of the spectral grid. Warnings are issued if the grid gets very large.
- (v14.0) Added checks for large inconsistencies with Saha equilibrium. This may be useful in identifying cases that have runaway solutions due to the aforementioned inconsistency in T_e.
- (v14.0) Intensity.in can be specified (applies a defined spectral radiance at the first line of sight point).
- (v14.0) Emissivity.in can be specified (applies emissivity/reflectivity at final point in the line of sight, e.g. optical property of the TPS).
- (v14.0) Two dimensional spectral radiance results can be output as a function of wavelength and distance.
- (v14.0) Non-local ‘escape factor’ calculation can be performed for atoms.
- (v14.0) Option for shock tube orientation calculation of radiance – perpendicular to line of sight.
- (v14.0) Ability to write atomic energy level populations.

6 Overall Structure of NEQAIR

The organizational structure of NEQAIR was significantly streamlined in the 2009-2013 timeframe. The main subroutine structure is as follows:

```
program neqair
    call MPI_init
    call readSpeciesNames
    call reorder_species
    call MPI_BCAST
    call BuildProcessMap
    call initialSetup
    call readLOS
    call setupLOS
    call distributeLOS
    call computeRadiation
       call compute_spectral_grid
       call MPI_BCAST
       call allocate_grid
       call atomic_populations
       call molecular_partition
       call molecular_populations
       call atomic_radiation
       call molecular_radiation
          call sort
          call setup
          call molecular_band
          call buildCDSDband
          call LineWidths
          call broadenband
          call ir_band
       call computeIrradiance
       call computeNormalLOS or computeShockTube
    call MPI_Finalize
```

7 Compiling the Code

There is a build script that is sent along with the NEQAIR distribution package. If the system that NEQAIR is to be run on has ifort (in the TSA division at NASA Ames Research Center, we are using ifort version 12.1.0) and mpif90 (in the TSA division at NASA Ames Research Center, we are using Open MPI version 1.4.4), the default build script should be able to run as is (except for maybe having to modify or delete the module load commands as fits your system). If it is necessary to modify or write a separate build script, it is necessary to force 8-byte reals (this is the –r8 flag in ifort), as many of the radiation equations will underflow for 4-byte reals and the MPI functionality in NEQAIR assumes 8-byte reals. Also, it has previously been established that using –fpe0 (i.e. capture floating point errors) can slow down the code on many systems. This is presumably due to error checking on the large number of exponentiations involved in the radiative calculations. NEQAIR has its own routines to capture or avoid these errors in places where they are likely to impact the result.

The build script itself has two flags that allows for compiling the code for different purposes. The code can be compiled to run serially with the flag -s, for users who do not have or want to use a cluster and/or MPI. Also, the code can be compiled in debug mode with the flag: -d. The debug mode is intended for development purposes and is used to diagnose failures in the code, and should run slower than the standard build. So it is only suggested to run the code in debug mode if you are experiencing an error, or if the code appears to be generating unexpected results. If you need help from the NEQAIR development team, it is recommended to try running the code using the debug compile first, so you can let the team know what the output is.

8 User Interface Updates

NEQAIR v14.0 should be back compatible with input files from NEQAIR2009v6 and onwards. Extra options have since been added to the input file, but this should not prevent earlier versions of the input file from working. Recent additions to the input file include: Scan Only, Saha-Boltzmann, atomic Argon, Infra-Red CO_2, Emissivity, Shock tube, Non-Local 'escape factor', 2-D output and the extra Slit Function Options. The format for the line-of-sight file (LOS.dat) has been kept the same.

9 Guide to NEQAIR Input Files

This section will run through the options available, and the files needed to run NEQAIR v14.0.

9.1 Overview of Required NEQAIR Data

For each line of sight point in the flow field, NEQAIR requires the distance, *x* in cm, temperatures, *Tt, Tr, Tv, Te*, in K (standard approach is to use *Te* = *Tv*) and the species number densities of each relevant species for the radiation calculation. A basic diagram of line of sight for NEQAIR is shown in Figure 1. These parameters are usually supplied by a CFD code.

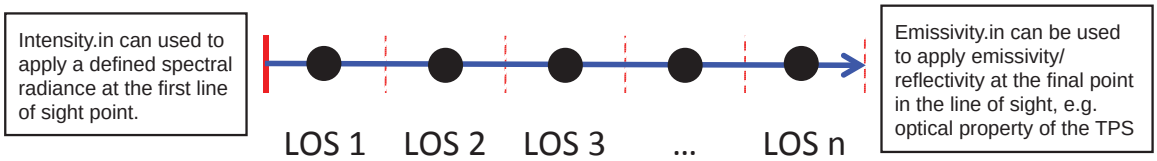


Figure 1. Diagram of basic line of sight for NEQAIR.

9.2 How to Run the Code

The best place to learn how to run the NEQAIR code is to start with the test cases. There are several test cases covering many atmospheres (such as Earth, Titan, Mars, Saturn and Venus). Copy the test case directory most relevant to your needs, and use the test case as a template for your run. The NEQAIR code will be executed by submitting the run_neqair.pbs script (specifically, the line: "`mpiexec -np $CPUS neqair > neqair.out`"). NEQAIR also requires two other files, neqair.inp and LOS.dat. These files are described in the following sections.

9.3 run_neqair.pbs

```
#PBS -S /bin/tcsh
#PBS -l walltime=00:05:00
#PBS -l nodes=3:ppn=24
#PBS -N fire2
#PBS -j oe
#PBS -q batch

limit stacksize unlimited

module load compilers/intel/intel-12
module load mpi/openmpi-1.4.4-intel64

cd $PBS_O_WORKDIR
set home = $PBS_O_WORKDIR
cd $home

rm -fr neqair.out

# Report when the job started
date

# Figure out how many nodes we're requesting--can use this later
set CPUS=`cat $PBS_NODEFILE | wc -l`

module load neqair/v14.0

# Run the program
mpiexec -np $CPUS neqair > neqair.out

# Report when the job finished
date
```

The pbs file has been updated to account for the parallelization of NEQAIR in v14.0. For best performance, the number of nodes and processors per node (ppn) requested for the job should multiply to equal (or be just greater than) the number of points in the LOS file minus one. This is specified in the line:

```
#PBS -l nodes=3:ppn=24
```

The optimum number of processes is equal to the number of points in the LOS file minus one (this is due to the first LOS point not be used in the radiation calculation, other than to define the starting x value). For example, for FIREII: 3 x 24 = 72 which is just greater than 72 – 1 = 71. In the event that there are not enough nodes available, it is recommended to have the number of nodes be greater than or equal to the largest possible fraction of this number, rounded up (e.g. 71/2 => 36 or 71/3 => 24 nodes for FIRE II).

The expected duration of the job is specified *hh*:*mm*:*ss* in the following line:

```
#PBS -l walltime=00:05:00
```

The name of the job as it will appear in the queue is specified with the following line:

```
#PBS -N fire2
```

The queue to which the job will be submitted to is specified with the following line:

```
#PBS -q batch
```

The batch queue is used to run many jobs, the long queue is used for jobs greater than 12 hours (should not be needed). The default queue can also be used if the number of jobs is less than 6.

NEQAIR is executed with the following line:

```
# Run the program
mpiexec -np $CPUS neqair > neqair.out
```

For the serial build of neqair, the following line may be used instead:

```
neqair > neqair.out
```

9.4 neqair.inp:

Most options in NEQAIR are selected by marking the appropriate location in neqair.inp with an 'X' or '0' (the number zero). In most cases, NEQAIR actually checks whether the character is a 0 or not, so if a letter 'O' or anything else other than a ‘0’ were entered, NEQAIR may consider the option selected.

```
*******************************************************************************
                        CEV Test Case
aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa <- 1st format line
1234567879 123456789 123456789 123456789 123456789 123456789
                                template.input

              Template of Input file for NEQAIR v14.0

     An unlimited number of comment lines can go here.

     The lines entered after the first line of ***'s above, and before the line
     of aaa's above will be printed as heading lines in the Output
     file.  Format for the heading lines is a70.

Line0
*******************************************************************************
```

Any comments added between the first “*****…” and “aaaaa…” is included in the header of the output file. Typically this is used as a case name. Additional comments, not included in the output, can be added into the input file between “aaaaa…” and “*********…”

```
PATH TO DATABASE FILES  :  /share/apps/neqair/v14.0/DATABASES/
Line2                                    a
-------------------------------------------------------------------------------
```

This specifies the location of the code's DATABASE files. The above is the DATABASE location maintained on redwood-2 and banyan.

```
PRINT OUT  :  Full Output X; Scan Only 0; 2D Data 0; Populations X;
Line3                    a            a          a               a
-------------------------------------------------------------------------
```

If Full Output is not ticked, intensity.out (the largest output file which contains the unconvolved high-resolution spectra) and LOS.out are not generated, and there is reduced output in neqair.out. If Scan Only is ticked, NEQAIR will look for the intensity.out file, and apply the spectral convolution scan as defined in neqair.inp – no radiative calculations will be performed. If 2D Data is selected, a 2-D matrix of output is generated against both wavelength and distance. When selecting 2D data, Full Output and/or Perform Scan (Line 9) must be selected, and the 2D data will be written to intensity.out and/or intensity_scanned.out, respectively. The 2D Data file may be very large (several GB) for Full Output, so this combination should only be selected if really necessary. If Populations is ticked, NEQAIR will output the species populations for the energy levels of all atoms included in the calculation. The output files will be listed as pop*XXX-YY*, where *XXX* is the number indicator for the point in the line of sight, and *YY* corresponds to the atomic species number in the NEQAIR input file.

```
KIND OF FLOW :nonBoltzmann X; d=    1.0; Boltzmann 0; BlackBody 0; Saha 0
Line4                      a    rrrrrr            a            a       a
-------------------------------------------------------------------------------
```

This line specifies how to calculate the excited state populations in the radiance calculation, as well as including options for generating blackbody spectra. In general, states may be calculated as a Boltzmann distribution, via the Quasi-Steady State (QSS) approximation or by the Saha equation. Not all of these options are available for all species. The distributions applied in a NEQAIR simulation by using the different input options is summarized in Table 2 and each distribution is plotted for a representative condition with atomic nitrogen in Figure 2. The example shown in Figure 2 is for an expanding flow, i.e. Saha > Boltzmann, (opposite trend compared to compressing flows).

Table 2. NEQAIR input/output combinations

INPUT OPTIONS				INPUT PARAMETER	OUTPUT				
Non-Boltzmann	Boltzmann	Blackbody	Saha	Definition of d	N2, O2, N2+, NO, CN, CO	Other Molecules	N, O, C	Other Atoms	Blackbody Applied at (if Black Body option selected)
X	0	0 or X	0	Esc dist (cm)	QSS	Boltz	QSS	Boltz	1st LOS Point
X	0	0 or X	X	Esc dist (cm)	QSS	Boltz	Saha	Saha	1st LOS Point
0	X	0 or X	0	N/A	Boltz	Boltz	Boltz	Boltz	1st LOS Point
0	X	0 or X	X	N/A	Boltz	Boltz	Saha	Saha	1st LOS Point
0	0	X	0	T (K)	N/A	N/A	N/A	N/A	Output

The first row is the most common set of inputs used with the Blackbody option not activated. All other combinations will produce an error.

In non-Boltzmann mode, a characteristic distance must be specified for escape factor calculations. This is given as the value 'd'. (Typically, 1.0 cm is used. Generally, this should be the same order of magnitude as the shock-standoff distance). For any radiance calculation, other than Blackbody, one of Boltzmann or non-Boltzmann must be selected.

The Blackbody calculation, if selected, operates in one of two modes. If Boltzmann and Non-Boltzmann are not selected, a Blackbody radiance is generated using the value assigned to “d” as the temperature (in K). If either Boltzmann or Non-Boltzmann is selected however, the first LOS point is treated as though it is radiating at a BlackBody defined by the temperature T_t at the first LOS point.

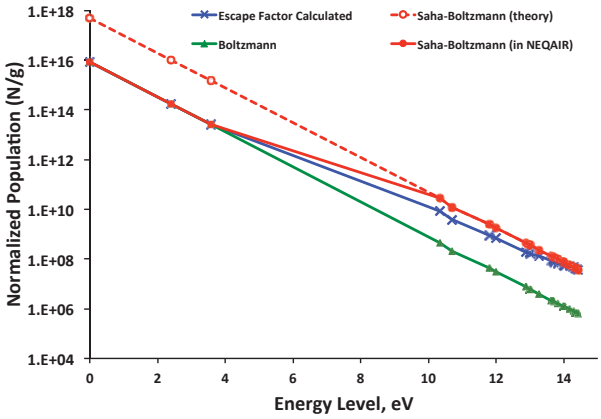


Figure 2. Various populations available in NEQAIR.

```
TYPE OF GEOMETRY : Line-of-Sight 0;  Stag Point X;  Shock Tube 0
Line5                             a              a              a
-------------------------------------------------------------------------------
```

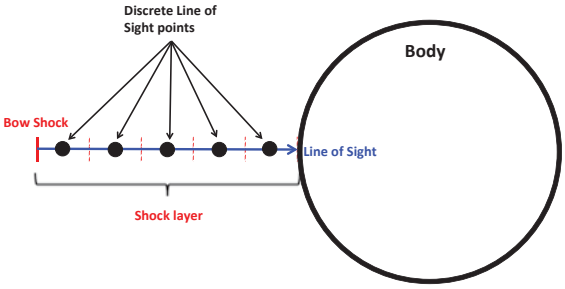
If Line-of-Sight is selected, NEQAIR will calculate the spectral radiance, see Figure 3a. If Stag Point is selected, NEQAIR will calculate the spectral radiance and the wall-directed heat flux, see Figure 3b. If Shock Tube is selected, the radiance will be calculated perpendicular to the line of sight, using a constant slab of width given by “d” (typically this would be the shock tube diameter), see Figure 3c. The results will be found in LOS.out with the radiance being integrated over the wavelength regions specified in neqair.inp. If 2D is selected, the spectral radiance may be found in intensity.out or intensity_scanned.out as a function of line of sight position. Unlike the other geometries, the first LOS point is calculated in Shock Tube geometry.

```
FOR STAG PT. :Infinite Slab X; Sphere. Cap 0;  Rnose=  0.0 cm;  Shock Div= 0.0
Line6                        a              a         rrrrrr               rrrrrr
-------------------------------------------------------------------------------
```

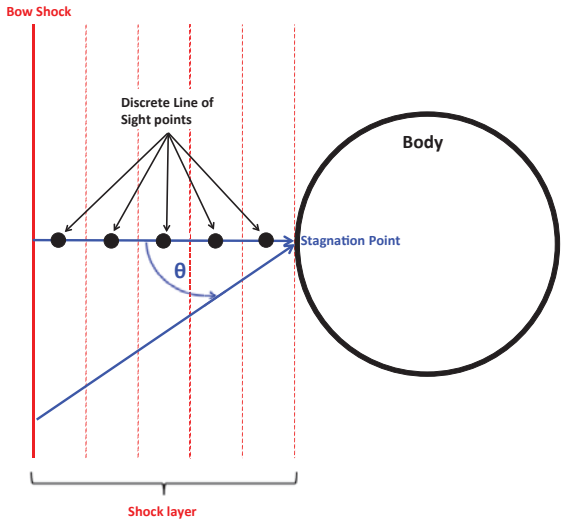
If Infinite Slab is selected, the tangent slab approximation is made. If the Spherical cap model is used, see Figure 3d, the following information is also required:

- *shock radius* = *Rnose* + *delta* + *shockdiv***phi* where
  - *Rnose* is the effective radius of body at stagnation point [cm],
  - *delta* is the shock standoff distance [cm] (calculated from the LOS file),
  - *shockdiv* is the shock divergence [cm/radian]
    - *shockdiv* = 0.0 specifies that the shock wave is concentric with body.

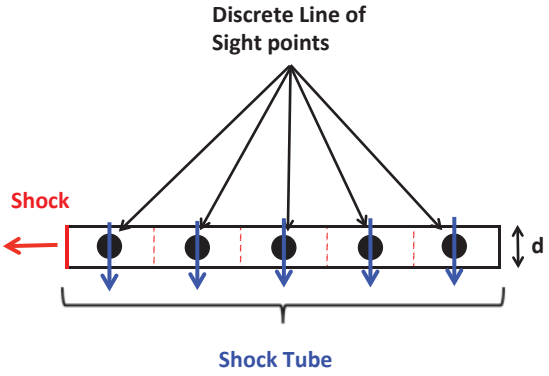
- *phi* is the angle between the stagnation streamline and a ray from the center of the spherical nose [radian].



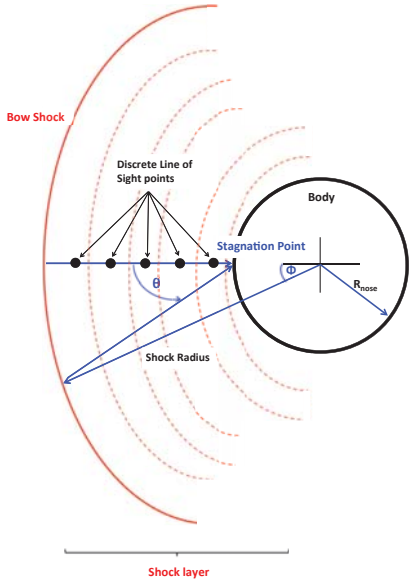
(a) Line of Sight



(b) Stag Point



(c) Shock Tube



(d) Spherical Cap

Figure 3. Different geometry options available in NEQAIR.

```
SYSTEMS      :Spectral Systems in Spectrum
Line7
             :Atomic Systems
              Escape Factors= Calculated X  or   0.0, NonLocal 0
                                           a     rrrrr           a
     Atom     smf:b-b        smf:b-f         smf:f-f
     N           1.0            1.0             1.0
     O           1.0            1.0             1.0
     C           0.0            0.0             0.0
     H           0.0            0.0             0.0
     He          0.0            0.0             0.0
     Ar          0.0            0.0             0.0
                 0.0            0.0             0.0  :End with blank and 0.0's.
     aaaaaaaa  rrrrr          rrrrr           rrrrr
```

For non-Boltzmann atomic calculations, the escape factor can be evaluated by the code by putting an X next to “Calculated” (this is the most common approach). Otherwise, if this is set to 0, the escape factor can be defined in the field after “or” in the range from 0 to 1. Note that specifying a value for the escape factor means the value for *d* in Line 4 is not used in the calculation.

Exact radiative transport calculations are complicated due to the coupled nature of the emitted and absorbed photons from each of the line of sight points. The radiation emitted and absorbed at every point in the flow field is coupled to the radiation emitted and absorbed at every other point. If NonLocal is selected, NEQAIR will iteratively calculate the level of excitation through the line-of-sight for atomic radiation, and therefore not need an escape factor, see Figure 4. This method uses a tangent slab approximation over the direction of the line of sight and T_t from the last line of sight point is used as the wall temperature. This plus the emissivity is used to calculate the boundary condition for the reverse flux (NonLocal calculation only) The NonLocal answer should be more correct, as fewer assumptions are made. However, the NonLocal solution may take significantly longer and may not make a noticeable impact to results. To quickly determine if running the NonLocal calculation is worthwhile,

examine the output obtained with the escape factor set to 0 and 1: the NonLocal result should lie between these two values. To improve the time required for the NonLocal calculation, Full Output and Perform Scan can be turned off. This way, the iteration is only converged on the total wall directed heat flux, and not the spectral radiance at each wavelength. Non-local may be performed in shock tube mode: the result still uses tangent slab along the line of sight. In this case, the first LOS point is treated as having zero radiance and the boundary after the following point is treated according to the emissivity selection (see below).

Each atomic transition, either bound-bound, bound-free, free-free can be turned on or turned off by setting the SMF to either 1 or 0 respectively. Note that free-free data is not available for all species. Values other than 1.0 will activate the mechanism, but does not rescale their magnitudes as in older versions of NEQAIR. If a species is activated but not included in the LOS.dat file, an error will occur.

Figure 4. Two way radiative heat flux.

```
For non-local calc, specify surface : E 1.00, T 0.00 (note: A=E, R=1-E-T)
     (E=emissivity, T=transmittance)    rrrr    rrrr
           :Diatomic Electronic Transition Systems
```

The Emissivity and Transmittance values are used in the NonLocal calculation. Furthermore, if the emissivity is set to a value of less than 1, the value of wall directed flux that is absorbed is also calculated and displayed in the neqair.out file. If an emissivity.in file exists, these values will be replaced by the content of that file.

Some relevant definitions:

E = emissivity: the relative ability of its surface to emit energy by radiation. It is the ratio of energy radiated by a particular material to energy radiated by a black body at the same temperature.

T = transmittance: the fraction of incident light that passes through a sample.

A = absorptivity: the ratio of the radiation falling upon a material to the radiation absorbed by the material. Thermodynamic principles require that absorptivity and emissivity are equal.

R = reflectivity: the fraction of incident radiance that is reflected or scattered at the surface.

```
                                                Major
                        One Band   SpinMult Branches vvExtend  Nmax
     Diatomic    smf  YN (vu,vl)  Use Real  Only!    [Ang's]
     --------- ---- ----------- --------  -----    -------  -----
  1  N2+ 1-     1.0   0 ( 0, 0)   1   2      X         0.0      0
  2  N2 1+      1.0   0 ( 0, 0)   1   3      X         0.0      0
  3  N2 2+      1.0   0 ( 0, 0)   1   3      X         0.0      0
  4  N2 BH2     0.0   0 ( 0, 0)   1   1      X         0.0      0
  5  NO beta    1.0   0 ( 0, 0)   1   2      X         0.0      0
  6  NO gam     1.0   0 ( 0, 0)   1   2      X         0.0      0
  7  NO del     0.0   0 ( 0, 0)   1   2      X         0.0      0
  8  NO eps     0.0   0 ( 0, 0)   1   2      X         0.0      0
  9  NO bp      0.0   0 ( 0, 0)   1   2      X         0.0      0
 10  NO gp      0.0   0 ( 0, 0)   1   2      X         0.0      0
 11  O2 SR      1.0   0 ( 0, 0)   1   3      X         0.0      0
 12  CN VIO     0.0   0 ( 0, 0)   1   2      X         0.0      0
 13  CN RED     0.0   0 ( 0, 0)   1   2      X         0.0      0
 14  CO 4+      0.0   0 ( 0, 0)   1   1      X         0.0      0
 15  C2 Swan    0.0   0 ( 0, 0)   1   3      X         0.0      0
 16  OH A-X     0.0   0 ( 0, 0)   1   2      X         0.0      0
 17  H2 B-X     0.0   0 ( 0, 0)   1   1      X         0.0      0
 18  H2 C-X     0.0   0 ( 0, 0)   1   1      X         0.0      0
 19  H2 B'-X    0.0   0 ( 0, 0)   1   1      X         0.0      0
 20  N2 LBH     0.0   0 ( 0, 0)   1   1      X         0.0      0
 21  N2 BH1     0.0   0 ( 0, 0)   1   1      X         0.0      0
 22  N2 WJ      0.0   0 ( 0, 0)   1   1      X         0.0      0
 23  N2 CY      0.0   0 ( 0, 0)   1   1      X         0.0      0
                0.0   0 ( 0, 0)   0   0      0         0.0      0:End Line
     aaaaaaaa rrrrr   a  ii ii    i   i      a      rrrrrr    iii

:Diatomic Infra-Red Transition Systems

                                               Major
                        One Band   SpinMult Branches
     Diatomic    smf  YN (vu, vl) Use Real  Only!
     --------- ---- -----  ----------- --------
  1  NO         0.0   0 ( 0, 0)   1   2      X
  2  CN         0.0   0 ( 0, 0)   1   2      X
  3  CO         0.0   0 ( 0, 0)   1   1      X
  4  OH         0.0   0 ( 0, 0)   1   2      X
  5  NH         0.0   0 ( 0, 0)   1   3      X
  6  CH         0.0   0 ( 0, 0)   1   2      X
  7  H2O        0.0   0 ( 0, 0)   1   2      X
  8  CO2        0.0   0 ( 0, 0)   1   2      X
                0.0   0 ( 0, 0)   0   0      0:End Line
     aaaaaaaa rrrrr   a     a  ii ii    i   i      a

Actual spin mult. does not need to be entered, it is informational only.
 Bands with origins from w1-vvExtend to w2+vvExtend of the wavelength range
 w1-w2 are included. Enter vvExtend=0.0 to include all bands.
 Nmax limits the number of rotational lines; enter 0(zero)to keep all rot lines.
```

The ipeak variable is no longer used in v14.0, as the performance enhancement it offered was negligible and for some cases it would eliminate meaningful radiance. As with the atomic transitions, all the molecular transitions can be activated or turned off by setting the SMF to either 1 or 0 respectively. (Note that using a value other than 1.0 will multiply the band strength by that value). The “One Band” option can be used to specify one specific vibrational band from any band system. To use the “One Band” option, YN must be selected for the appropriate transition (i.e. set to ‘X’), then specify vu, and vl. The spin multiplicity numbers are legacy inputs that should not be adjusted (the "use" column was intended to allow selecting whether or not spin multiplicity be treated explicitly. Setting these to a larger value increases the molecular radiance to levels inconsistent with validation data. The "actual" column is purely informational). The Major Branches Only option will ignore forbidden bands when selected. Generally this option

has little to no impact on run-time or output. The vvExtend option has been disabled in v14.0 (previously vvExtend eliminated vibrational bands which lay beyond the domain set in Region Data - this had little benefit to run time and was seldom used). Nmax, if set to a number other than zero, may be used to limit the maximum rotational quantum allowed in the calculation. Generally, this should be set to 0.

```
REGION DATA:        Line8                    # of regions =  4
                                                            iii
   w1 [A]   w2 [A]   range   grid_type  delta_lambda   pointsPerLine
   855.5   2000.0     600        1        0.00133          10
  2000.0   6350.0      50        1        0.00334          10
  6350.0  16000.0      50        1        0.01135          10
 16000.0  39600.0      25        1        0.03806          10
 rrrrrrr  rrrrrrr    iiii        i        rrrrrrr          iii
```

# of regions must be set to the number of spectral regions broken up by wavelength. For each region, a start and end wavelength must be defined, w1 and w2. Note that NEQAIR expects the regions to be in order and continuous. Additionally, radiance calculated in one region is not broadened into adjacent regions, so that the region boundaries should be chosen to lie in areas of the spectrum without significant features. Range specifies how far out to calculate line broadening, specified as a multiple of the line width. If 0 is entered, NEQAIR will carry out the broadening until it is too weak to have an impact to the spectrum or the end of the region is reached. Commonly used values based on the wavelength range are shown above. If grid_type 1 is used, the minimum spacing required for each region is calculated by NEQAIR, based on the properties of the 2nd LOS point. In this case, pointsPerLine specifies the minimum number of grid points to use for each line. If grid_type 0 is used, the delta_lambda value is used for the grid spacing for each region.

```
SCAN DATA:          Line9        Perform Scan X
                                            a
Slit Function (Voigt,ICCD1,etc) : Voigt    Spectral interval [A] = 0.1
                                  aaaaaa                           rrrrr
Slit Parameters:
      6.0   0.0     2.0       Voigt
      6.0   0.0     2.0       Voigt
      6.0   0.0     2.0       Voigt
      6.0   0.0     0.0       Voigt
 widthg[A], widthl[A], range , SlitFn (optional)

Notes:
Allowed slit functions are Voigt, ICCD1, ICCD2, or SGauss
Spectral interval of 0 means it is auto-selected as 1/10th of linewidth
For Voigt, SGauss and ICCD1, range determines how wide to make the scan function
        If range>1 it is the number of half-widths to scan
        If range<1 it is the fraction of peak value to include
        If range=0 NEQAIR picks the range itself
The ICCD1 scan function is defined as sqrt(Voigt)
For ICCD2, the scan function is defined as
                I(x) = [G(wg,x)+r*L(wl,x)]/(1+r)
        where G and L are Gaussian and Lorentzians with widths wg, wl
        and r = 10^range
The extent of the scan function to use is determined automatically for ICCD2
SGauss is a smeared Gaussian:
        Input parameters are Gaussian and Smearing components (in A)

Everything from here on down is ignored

--------------------------------------------------------------------------------
```

This last section describes the spectral scanning of the calculated spectral intensity. If Perform Scan is set to 0, no scan is performed. If Perform Scan is set to X, the results in intensity.out will be scanned based on the specified settings. There are several options for the slit function: Voigt, SGauss, ICCD1, ICCD2 (all of which are described in the text at the end of the input file). The Slit function can either globally be defined after Slit Function, or defined for each spectral region. The Spectral Interval needs to be defined in terms of increments in angstroms. Each spectral region then needs the Gauss and Lorentzian widths along with a range value. The range value is also described in the text at the bottom of the input file.

9.5 LOS.dat

The LOS.dat file contains information regarding the line-of-sight information which NEQAIR uses for the radiation calculation. The file details the species in the line of sight and includes the x location in cm, the translation, rotation, vibration, electron/electronic temperatures in K and the species number densities in $1/cm^3$. The shock location is defined at the start of the LOS file, then increasing in x until reaching the body location at the final point. More detailed information on LOS.dat can be found in the header of the file. The starting x-location is defined by the x coordinate specified in the first LOS point. The temperatures and number densities in the first LOS point are not used in the calculation, except when BlackBody or ShockTube are selected. Species that NEQAIR does not recognize for radiation calculations can be specified in LOS.dat in the present version of the code – previously, this would've caused an error. For shock to body calculations, it is advisable that the first LOS point have a vibrational temperature of at least 500 K.

```
*****************************************************************************
                    LOS file for EAST MWIR CO2 Test Case

       An unlimited number of comment lines can go here.

       Enter Data AFTER the data-format lines!

   (1) Enter species in any order; limited to atoms, diatomics, triatomics,
       atomic ions, diatiomic ions, and electrons. Left-justify the species
       symbols in the fields.  Dimensioned up to 25 species.  End entry
       with a blank line.

   (2) Properties entered at each grid point along line-of-sight.  The
       properties apply to the layer between the grid point and the
       previous grid point.  Thus, the properties at the first grid point
       are not used.  This grid point only establishes the origin of the
       line-of-sight.

   (3) Enter species number densities [cm-3] in the same order that the species
       symbols are entered.  End data entry at each grid point with a blank
       line.

   (4) End line-of-sight data entry, with a line of 0's as shown.

*****************************************************************************
         aaaaaaaa       aaaaaaaa       aaaaaaaa       aaaaaaaa    (2x,(7x,a8))
         CO2            CO             N2             O2       :Species Symbols.
         NO             N              O

-----------------------------------------------------------------------------
   no.   x,cm   total partcc       t        tr        tv        te  (i5,f8.3,
iiiii rrrrrrr rrrrrrrrrrrrr rrrrrrrr rrrrrrrr rrrrrrrr rrrrrrrrre15.6,4f10.1
       rrrrrrrrrrrrr rrrrrrrrrrrrr rrrrrrrrrrrrr rrrrrrrrrrrr   (6x,4e15.6)
       Include these 9 lines (from --- to --- lines) for first grid point only!!
       End each grid point entry with a blank line.
       End data file with a line of zero's as shown on the next line.
    0     0.0            0.0       0.0       0.0       0.0       0.0
-----------------------------------------------------------------------------
    1  0.0000000E+00  8.0266E+17    2978.84   2978.84   2978.84   2978.84
        2.5214000E+17  3.3091000E+17  2.1256000E+16  1.3256000E+17
        6.0713000E+15  2.7567000E+12  5.9713000E+16

    2  1.0160000E+01  8.0266E+17    2978.84   2978.84   2978.84   2978.84
        2.5214000E+17  3.3091000E+17  2.1256000E+16  1.3256000E+17
        6.0713000E+15  2.7567000E+12  5.9713000E+16

    0     0.0            0.0       0.0       0.0       0.0       0.0
```

9.6 Optional Input Files

9.6.1 Intensity.in

The values specified in intensity.in apply a defined spectral radiance at the first line of sight point, for calculations performed in the direction of the LOS. The rules for the format of intensity.in are as follows: Headers cannot begin with numbers, but are otherwise unlimited, the first column is wavelength (in Angstroms), the third column is radiance (in W/cm^2 μm sr). The reason for this is that the optically thick output is displayed in the 3rd column for intensity.out, thus allowing an intensity.out from one simulation to be copied to intensity.in without modification. NEQAIR will use the 2nd column as radiance if there is no 3rd column specified in intensity.in – this is useful for creating an intensity.in from sources other than NEQAIR.

9.6.2 Emissivity.in

The total wall directed heat flux absorbed at the surface is calculated based on the data in emissivity.in, and is displayed in neqair.out. This may also be used in a non-local calculation. The rules for the format of emissivity.in are the same for intensity.in: Headers cannot begin with numbers, but are otherwise unlimited, the first column is wavelength (in Angstroms), the second column is emissivity (same as absorptivity) and the third column is reflectivity. Specifying reflectivity is optional, if it is not specified NEQAIR assumes r = 1 – e (i.e. no transmission).

10 Guide to NEQAIR Output Files

10.1 Various Mechanisms Identified in Output

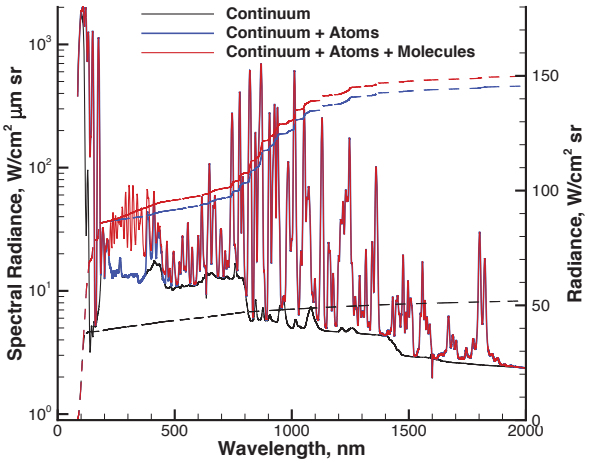


Figure 5. Different components of spectral radiance.

10.2 intensity.out

This file has the final unconvolved spectra that has been transported through the entire line-of-sight specified in LOS.dat. The data in the file consist of the wavelength in Å, the optically thin spectral radiance in W/cm^2 μm sr, the optically thick spectral radiance in W/cm^2 μm sr and the cumulative integral of this last value (radiance, W/cm^2-sr). This file is useful for a very thorough comparison of two computed spectra. An example of this output is shown in Figure 6.

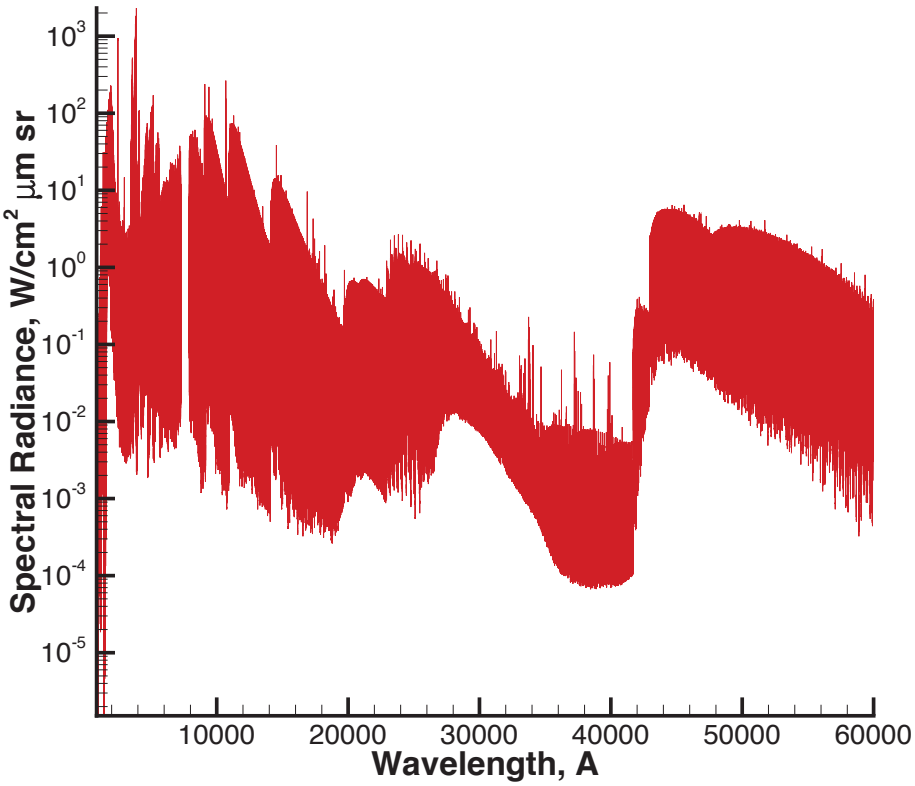


Figure 6. intensity.out for the NEQAIR Mars test case.

10.3 intensity_scanned.out

This file has the final convolved spectra that has been transported through the entire line-of-sight specified in LOS.dat. The convolution information is declared in neqair.inp. The data in the file consist of the wavelength in Å, the optically thick spectral radiance in W/cm^2 μm sr, and the integral of this value (i.e. radiance, W/cm2-sr). This file is useful for comparisons with experimental spectra (particularly when the instrument convolution function is well known). The intensity_scanned.out file can also be used to observe what the predominant radiating transitions are. An example of this output is shown in Figure 7.

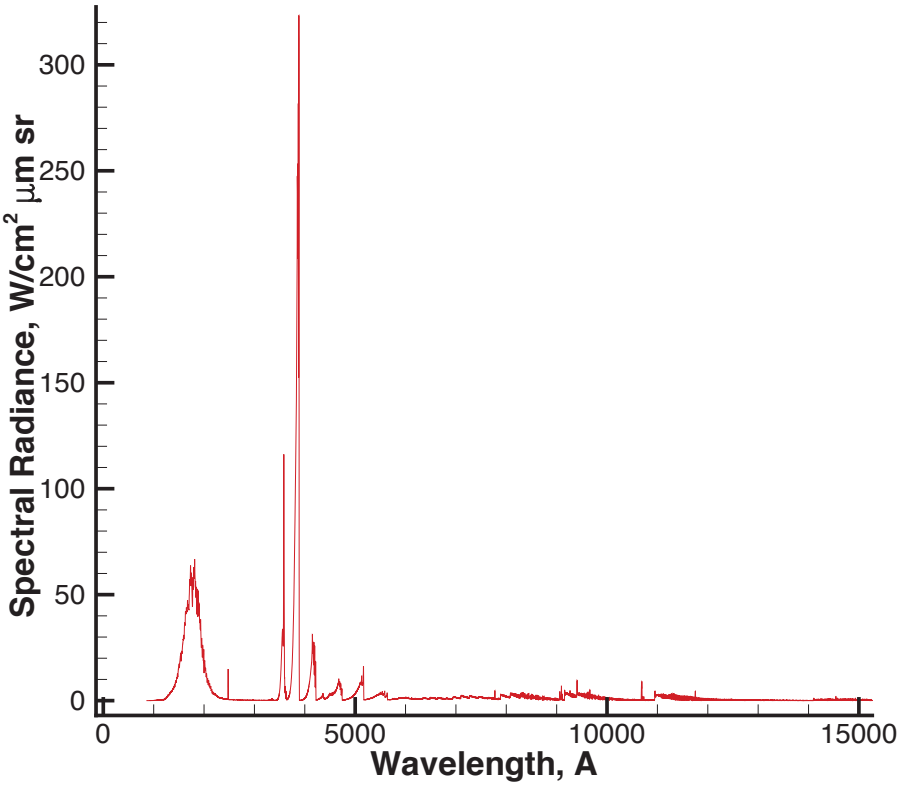


Figure 7. intensity_scanned.out for the NEQAIR Mars test case.

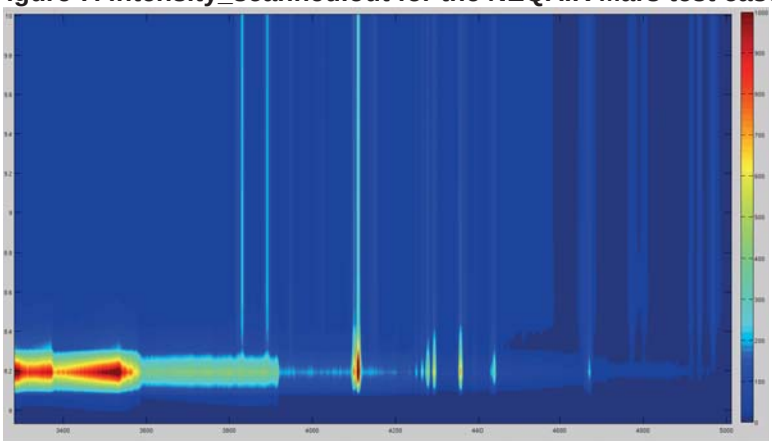


Figure 8. 2-D intensity_scanned.out for high speed Earth entry

10.4 LOS.out

The LOS.out file contains the radiance as a function of distance, along the normal line of sight. This file can be helpful to determine which parts of the flowfield are radiating or absorbing. The file contains the distance in cm, the total radiance in W/cm^2 sr, followed by a breakdown of the radiance by the regions specified in neqair.inp. An example of this output is shown in Figure 9.

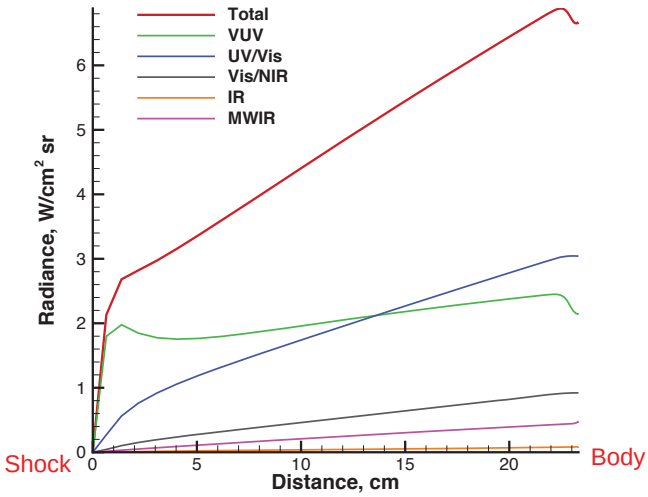


Figure 9. LOS.out for the NEQAIR Mars test case.

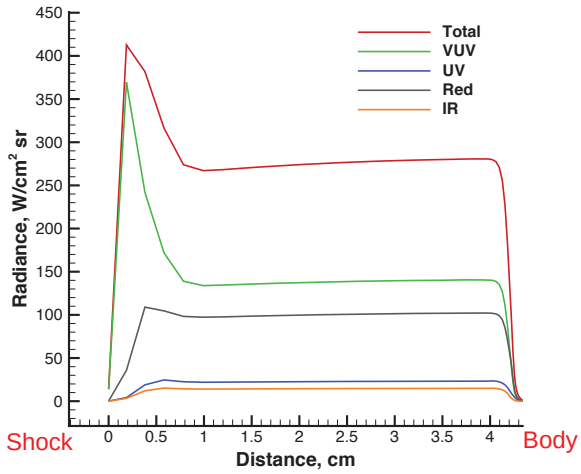


Figure 10. LOS.out for the NEQAIR for the FIRE II test case (in shock tube mode).

10.5 neqair.out

While this NEQAIR output is written to standard out, it is often useful to redirect this output to a file. In the NEQAIR distribution package it is written to neqair.out as specified by the following line in run_neqair.pbs:

```
# Run the program
mpiexec -np $CPUS neqair > neqair.out
```

The filename “neqair.out” can be changed to anything the user would like. If Full Output is selected (as is in the example given below) the file gives information regarding the neqair run, e.g. what parameters and radiating transitions were included.[2] The final total radiative heating value is given on the last line. This value is provided even if Full Output is set to off.

Mars Test Case.

STANDARD OUTPUT FOR NEQAIR

Line 1; A Spectrum was Created AND Scanned.
Line 2; Database file path = /share/apps/neqair/v14.0/DATABASES/
Line 3; Full output will be written to standard output
Line 4; Radiation is for NonBoltzmann Excitation.
Line 5; This is a Stagnation Point Case.
Line 6; The Stagnation Point Flow is modeled as an Infinite Slab
Line 7; Spectral Systems and Parameters

Atomic Systems

Line 10; All b-b atomic Escape Factors are calculated locally.

	Atom	smf:b-b	smf:b-f	smf:f-f
1	N	1.00	1.00	1.00
2	O	1.00	1.00	1.00
3	C	1.00	1.00	1.00

Diatomic Electronic Transition Systems

	Diatomic	smf	One Band YN (vu, vl)	SpinMult Use	SpinMult Real	Major Branches Only!	vvExtend [angstrom]	Nmax
1	N2 1+	1.00	0 (0, 0)	1	3	X	0.0	0
2	N2 2+	1.00	0 (0, 0)	1	3	X	0.0	0
3	N2 BH2	1.00	0 (0, 0)	1	1	X	0.0	0
4	NO beta	1.00	0 (0, 0)	1	2	X	0.0	0
5	NO gam	1.00	0 (0, 0)	1	2	X	0.0	0
6	NO del	1.00	0 (0, 0)	1	2	X	0.0	0
7	NO eps	1.00	0 (0, 0)	1	2	X	0.0	0
8	O2 SR	1.00	0 (0, 0)	1	3	X	0.0	0
9	CN VIO	1.00	0 (0, 0)	1	2	X	0.0	0
10	CN RED	1.00	0 (0, 0)	1	2	X	0.0	0
11	CO 4+	1.00	0 (0, 0)	1	1	X	0.0	0
12	C2 Swan	1.00	0 (0, 0)	1	3	X	0.0	0

Diatomic Infra-Red (IR) Transition Systems

	Diatomic	smf	One Band YN (vu, vl)	SpinMult Use	SpinMult Real	Major Branches Only!
1	CN	1.00	0 (0, 0)	1	2	X
2	CO	1.00	0 (0, 0)	1	1	X
3	CO2	1.00	0 (0, 0)	1	0	X

```
          Line 8; Wavelength Regions

 region   w1        w2      range grid_type deltaLam  nPointsPerLine

    1    855.50   2000.00    600      1    0.0013     10
    2   2000.00   5800.00     50      1    0.0033     10
    3   5800.00  16000.00     50      1    0.0114     10
    4  16000.00  39600.00     25      1    0.0381     10
    5  39600.00  60000.00     25      1    0.0381     10

 Completed CDSD ReadIn
 Reading TOPBase b-f data for C
 Reading TOPBase b-f data for N
 Reading TOPBase b-f data for O

Region 1 number of equispaced grid points =       825568
Region 2 number of equispaced grid points =      1149352
Region 3 number of equispaced grid points =      1013631
Region 4 number of equispaced grid points =       837191
Region 5 number of equispaced grid points =       265320

Warning: ne of 6.8E+03 is more than 100x greater than the Saha limit at  2002 K
Warning: ne of 3.2E+12 is more than 100x greater than the Saha limit at  2466 K
Warning: ne of 4.8E+12 is more than 100x greater than the Saha limit at  2780 K
Warning: ne of 8.2E+11 is more than 100x greater than the Saha limit at  2098 K
Warning: ne of 2.0E+12 is more than 100x greater than the Saha limit at  2259 K
Warning: ne of 3.7E+12 is more than 100x greater than the Saha limit at  2557 K
Warning: ne of 2.8E+12 is more than 100x greater than the Saha limit at  2386 K
Warning: ne of 2.4E+12 is more than 100x greater than the Saha limit at  2318 K
Warning: ne of 1.2E+11 is more than 100x greater than the Saha limit at  2016 K
Warning: ne of 2.6E+11 is more than 100x greater than the Saha limit at  2031 K
Warning: ne of 6.1E+11 is more than 100x greater than the Saha limit at  2072 K
Warning: ne of 1.1E+12 is more than 100x greater than the Saha limit at  2129 K
Warning: ne of 6.2E+12 is more than 100x greater than the Saha limit at  3059 K
Warning: ne of 1.6E+12 is more than 100x greater than the Saha limit at  2208 K
Warning: ne of 4.2E+12 is more than 100x greater than the Saha limit at  2662 K
Warning: ne of 4.2E+11 is more than 100x greater than the Saha limit at  2050 K
Warning: ne of 5.5E+12 is more than 100x greater than the Saha limit at  2913 K
Warning: ne of 7.1E+12 is more than 100x greater than the Saha limit at  3219 K
Warning: ne of 1.3E+12 is more than 100x greater than the Saha limit at  2166 K
Radiative heating from   855.50 to  2000.00 angstroms =  0.791184E+01 W/cm2
Radiative heating from  2000.00 to  5800.00 angstroms =  0.166056E+02 W/cm2
Radiative heating from  5800.00 to 16000.00 angstroms =  0.560963E+01 W/cm2
Radiative heating from 16000.00 to 39600.00 angstroms =  0.516452E+00 W/cm2
Radiative heating from 39600.00 to 60000.00 angstroms =  0.240512E+01 W/cm2


Total radiative heating from    855.50 to  60000.00 angstroms =    33.048661 W/cm2
```

10.6 Populations Output (pop*XXX*-*YY*)

If populations is selected in the NEQAIR input file, NEQAIR will output the species populations for the energy levels of all atoms included in the calculation. The output files will be listed as pop*XXX*-*YY*, where *XXX* is the number indicator for the point in the line of sight, and *YY* corresponds to the atomic species number in the NEQAIR input file. The format of the file is to list the Energy Level in cm^{-1}, the normalized population (N/g) and the degeneracy (g). This can be used to generate a Boltzmann plot, similar to what was shown in Figure 2. At the end of the file, the ionization potential, the Saha normalization and Ion number density is also listed.

11 Usage Recommendations/Notes

11.1 For CFD used as input to NEQAIR

As has been mention several times in this report, it is highly beneficial for NEQAIR to have input from CFD that has used $T_{electrons} = T_{vibration}$. Non-physical answers can be obtained if $T_{electrons} = T_{translation}$ (under certain conditions, the answer can be several orders of magnitude higher than it should be). Furthermore, it is suggested that the CFD calculation be run with electrons in the flowfield. If electrons are not used, a minimum value of 1000 parts/cm^3 will be assumed in order for aspects of NEQAIR to run, e.g. the non-Boltzmann QSS calculation.

11.2 Scanning Spectra

If glitches in the scanned spectra are observed on the edges of the spectral regions defined in neqair.inp, this is an artifact of the scanning routine conserving the area under the curve from the unconvolved spectrum. For the best results, the region boundaries should be placed in regions with minimal spectral radiance. If a particular spectral region needs to be examined, the regions defined in neqair.inp can be increased slightly on both sides to avoid the possibility of the glitch appearing in the spectral region of interest.

11.3 Which Grid Type to Use

The default grid type to use is grid_type 1. This will mean that the grid spacing is defined by NEQAIR. However, if the calculation appears to take longer than expected (possibly indicated with the message, “WARNING: number of grid points is exceptionally large…”). The grid_type can be set to 0. This means that the user defines the spectral spacing. It is recommended to compare the results obtained with grid_type 0, with the results obtained with grid_type 1 to confirm that the grid spacing has not been increased so large that the spectral lines are no longer well defined. Alternatively, a grid resolution study may be performed to confirm the resolution is high enough to accurately capture the heating magnitude. Further information can be found in the section: “Description of NEQAIR Warning and Error Messages”.

11.4 Venus Radiation

The C bound-free from TOPBase implemented in NEQAIR has not yet been fully validated with experiment, due to the lack of VUV data from EAST at conditions relevant to Venus entry. The TOPBase database has shown improved agreement with EAST for N and O bound-free compared to the previously implemented Peach cross-sections. However, preliminary comparisons with EAST indicate the TOPBase bound-free may offer an over-prediction of the spectral radiance in the VUV. The previous cross-sections of Peach appear to under-predict the data from EAST. Future experiments on EAST would be required to properly validate the data and/or update the cross-sections if necessary.

11.5 Expanding/Afterbody Flows

As there is no experimental data for radiation relevant to atmospheric entry encountered in afterbody flows, the NEQAIR results have not been well validated for such regimes. Differences on the order of a factor of 2 have been seen in the afterbody compared with other radiation codes.

11.6 Parsing CFD results to NEQAIR

CFD solutions tend to start with freestream conditions at low temperatures. When parsing the results to NEQAIR, it is recommended to only include the CFD results from when Tv becomes greater than approximately 500K (indicating the beginning of the shock). If the temperature is low at the first line of sight point, the grid can become excessively large and slow down the simulation. If the temperature is extremely low at the first point, errors or failures in the code can occur.

12 Performance Results

The following two tables list the performance of several recent versions of NEQAIR using the Redwood-2 cluster at NASA Ames, both in terms of the body directed radiative heat flux (Table 3) and in terms of the run time (Table 4). 13.1r2 is a version of 13.1 that contains a few small bug fixes in order to confirm results obtained with 13.2. 13.1r2 does not contain the additional physics included in 13.2.

Table 3. Radiance for NEQAIR test cases.

Radiative Heating, W/cm^2	CEV	MWIR Mars EAST Shot	FIREII	Mars	Titan	Venus	Saturn
2009v8	19.4	4.7	609.0	42.2	30.1	2795.0	308.5
v13.1	19.4	4.8	606.6	42.2	30.1	2852.9	308.3
v13.1r2				35.7		2962.0	257.7
v13.2	20.4	4.8	660.7	37.6	30.1	3776.0	258.7
v14.0	20.9	4.8	669.3	33.1	9.3	4000.8	262.1
Percent Difference:							
v8 -> 13.1	**0.1%**	**0.9%**	**-0.4%**	**0.0%**	**0.0%**	**2.0%**	**-0.1%**
13.1* -> 13.2	**4.7%**	**0.0%**	**8.2%**	**5.1%**	**0.1%**	**21.6%**	**0.4%**
* (r2 where appropriate)							
v13.2 -> v14.0	**2.7%**	**0.2%**	**1.3%**	**-13.5%**	**-224.3%**	**5.6%**	**1.3%**

Table 4. Run time's for NEQAIR test cases.

Number of points in LOS	78	1	71	58	70	57	118
Computational Time, minutes	**CEV**	**MWIR Mars EAST Shot**	**FIREII**	**Mars**	**Titan**	**Venus**	**Saturn**
v13.1	40	2.5	18	53	22.5	23.5	32
v13.1r2				53		16	28
v13.2	140	1.5	89	211.5	22	74	20
v14.0 (processors=#LOS)	2.4	1.1	1.9	4.9	0.9	2.5	0.9
v14.0 (1 processor)	56.8	1.1	35.4	82.0	13.6	46.8	23.7
Speed Up Factor (v13.2 -> v14.0)	**58**	**1**	**48**	**43**	**25**	**30**	**23**

12.1 Notes on Test Cases

Each test case directory contains the appropriate LOS.dat, neqair.inp and run_neqair.pbs files. They are located on Banyan and Redwood-2 at the following location:

/share/apps/neqair/v14.0-prerelease/TEST_CASES/

To run a test case, copy the directory to your local directory, and submit run_neqair.pbs.

Each test case directory also contains the output from several recent versions of NEQAIR.

The following two sections will detail the reasons for the differences in results for the test cases between the latest three versions of NEQAIR.

12.1.1 From v13.1 to v13.2

CEV: The small change in intensity is due to an increase in the nitrogen bound-free based on the TOPBase cross sections.

MWIR Mars EAST Shot: No significant change, as expected.

FIRE II: The change in intensity is due to an increase in the nitrogen bound-free based on the TOPBase cross sections, combined with a small error in QSS for the final LOS point. This error was fixed in v14.0.

Mars: A bug found was found in v13.1 when more than 1 IR band is turned on, this was fixed. The small increase from v13.2 compared to v13.1r2 is due to the C TOPBase cross sections and more atomic C lines in NIST 5.0.

Titan: No significant change, as expected.

Venus: Increase due to C TOPBase cross sections, appears to be validated against EAST for UV/Vis/NIR, but preliminary checks suggest it could be providing an over-prediction in VUV. More deep VUV validation data is required. Therefore, the Venus results from NEQAIR's current version could be providing an over-prediction.

Saturn: Bug found in v13.1 related to broadening. This was fixed, and no significant difference between v13.1r2 and v13.2 was found, as expected.

12.1.2 From v13.2 to v14.0

All test cases are faster in v14.0 when it is run with 1 processor compared to v13.2, but not quite as fast as v13.1. The longer computational run time for v13.2 and v14.0 is due to the significant increase in the size of the databases (particularly the TOPBase b-f data). The main advantage of v14.0 is that it can be run in parallel, which increases the computational time by about a factor of 10 compared to when the code is run serially. This is an increase of up to about 35 compared to v13.2, so is a substantial upgrade in computational time, while still capturing the fidelity of the larger databases. The parallel times can be seen in the table row listed as 'v14.0 (full nodes)'. "Full nodes" indicates that the number of nodes corresponds to the number of points in the line-of-sight file.

CEV, FIRE II, SATURN: The small change in intensity is due to a change in the tangent slab integration.

MWIR Mars EAST Shot: No change, as expected.

Mars: The decrease in the intensity is due to switching the test case to QSS. The increase due to the tangent slab integration and the increase from extending the wavelength region out to 60 000 Å offsets the decrease to a small extent.

Titan: The significant decrease in the intensity is due to switching the test case to QSS. The QSS for this case would not be able to run in v13.2, as it was below the minimum electron mole fraction permitted for QSS in that version.

Venus: The increase in intensity is due to a combination of the change in tangent slab integration, and the effect of removing the ipeak limiter, which culled molecular band branches based on optically thin intensity.

13 Bibliography

Brandis, A., Johnston, C., Cruden, B., Prabhu, D., & Bose, D. (2012). Validation of High Speed Earth Atmospheric Entry Radiative Heating from 9.5 to 15.5 km/s. *43rd AIAA Thermophysics Conference. AIAA 2012-2865.* AIAA.

Brandis, A., Johnston, C., Cruden, B., Prabhu, D., Wray, A., Liu, Y., et al. (2013). Validation of CO 4th Positive Radiation for Mars Entry. *Journal of Quantitative Spectroscopy and Radiative Transfer , 121*, 91-104.

Brandis, A., Wray, A., Liu, Y., Schwenke, D., Huo, W., & Johnston, C. (2013). Validation of HyperRad for Earth Entries. *44th AIAA Thermophysics Conference. AIAA 2013-2777.* AIAA.

Cunto, W., Mendoza, C., Ochsenbein, F., & Zeippen, C. (1993). TOPbase at the CDS. *Astronomy and Astrophysics , 275*, L5-L8.

Gilmore, F., Laher, R., & Espy, P. (1992). Franck-Condon factors, r-centroids, electronic transition moments, and Einstein coefficients for many nitrogen and oxygen band systems. *Journal of Physical and Chemical Reference Data , 21*, 1005.

Hyun, S. (2009). *Spradian07: Radiation Code Spradian07 and Its Applications.* PhD Thesis, KAIST.

Kramida, A., Ralchenko, Y., & Reader, J. (2012, July). *NIST Atomic Spectra Database, Version 5.0.0*. Retrieved November 2014, from http://physics.nist.gov/asd

Laux, C. (1993). *Optical diagnostics and radiative emission of air plasmas.* PhD Thesis, Stanford University.

Mazaheri, A., Gnoffo, P., Johnston, C., & Kleb, B. (2010). *LAURA Users Manual.* NASA Langley Research Center. TM 2010-216836.

Peach, G. (1970). Continuous Absorption Coefficients for Non-hydrogenic Atoms. *Memoirs of the Royal Astronomical Society , 73*, 1-123.

Tashkun, S., & Perevalov, V. (2011). CDSD-4000: High-Resolution, High-Temperature Carbon Dioxide Spectroscopic Databank. *Journal of Quantitative Spectroscopy and Radiative Transfer , 112* (9), 1403-1410.

Wright, M., White, T., & Mangini, N. (2009). *Data-Parallel Line Relaxation Methods (DPLR) Code User Manual Acadia-Version 4.01.1.* NASA Ames Research Center. Moffett Field: TM-2009-215388.

14 Description of NEQAIR Warning and Error Messages

WARNING: number of grid points is exceptionally large
Check neqair.inp and LOS.dat to determine if this is what you really want.

If you get this warning, there are 3 things that you might want to check. If the first point/s in LOS.dat start at very low vibrational temperatures (i.e. < 500 K), and grid_type is set to 1, the grid can become larger than required, therefore, it is recommended to delete the points up until the vibrational temperature passes 500 K. If grid_type is set to 0 and a very small delta_lambda has been used, you can try setting grid_type to 1, or alternatively you can try increasing delta_lambda. However, care must be taken in order to make sure that delta_lambda is not set so large that there will not be enough points to correctly describe each spectral line.

WARNING: QSS data not available for *xxx*

This indicates that there is no QSS data for the specified species, and NEQAIR will run the calculation with a Boltzmann distribution for this species.

WARNING: Stark broadening parameters not available for *xxx*

This warning will appear if atomic H or Ar are turned on, and lets the user know that an empirical Stark broadening has been applied to either H or Ar.

NEQAIR WARNING: Data for atomic *xxx* f-f radiation has not been entered

This warning will appear if the user selects H or He free-free. The warning lets the user know that free-free radiation from H and He is currently not included in NEQAIR.

WARNING: Can't use Saha equation at *t* K

This warning will appear if NEQAIR is set to run using Saha-Boltzmann and if the code identifies that there is a population inversion, the code will run using Boltzmann for that species and point in LOS.dat

WARNING: species *xxx* is not in LEVELS_ATOMS.dat database

This warning indicates that the specified atomic species has been requested in the LOS.dat file but is not a species supported by NEQAIR. In previous versions of NEQAIR, this was a fatal error and the code would stop.

WARNING: species *xxx* is not in LEVELS_MOLE.dat database

This warning indicates that the specified molecular species has been requested in the LOS.dat file but is not a species supported by NEQAIR. In previous versions of NEQAIR, this was a fatal error and the code would stop.

WARNING: The molecule for band system *xxx* is not in species list

This warning indicates that the specified molecular band system has been requested in the neqair.inp file but is not in LOS.dat.

Warning: ne of *xxx* is more than 100x greater than the Saha limit at *t* K

This warning indicates that the electron number density is far from Saha equilibrium and there is therefore a possibility that some processes will radiate at a much stronger

level than is physically realistic. This could be due to assumptions made in the CFD solver, before the data was ported over to NEQAIR. For example, DPLR typically assumes $T_e = T_t$ while NEQAIR is usually run with $T_e = T_v$, which can lead to inconsistent answers. Ideally, the CFD used to generate the line-of-sight data for NEQAIR should be run with $T_e = T_v$. In this situation, the user may want to verify whether the electron temperatures and densities in LOS.dat are realistic.

Error *xxx* not recognized in eqc

Eqc (called by the molecular QSS calculation) requires the populations both of the molecule, and the dissociated products, e.g. if CO is used, C and O would also be needed. Please check LOS.dat.

neqERROR: Overflow in optical depth

This error will occur if the optical depth (i.e. sum of absorbances x widths) goes beyond NEQAIR's ability to prevent data underflow (typically around 10^{12}) and is usually an indication of a non-physical result. If this error is seen, please check that your input in LOS.dat is correct, and in the correct units. If the data in LOS.dat came from a CFD solver, please check that the results were correctly ported over, with the appropriate unit conversions. If everything has been checked and the error still occurs, please contact the NEQAIR developers.

ERROR reading database path

The path to the database files indicated in the top of neqair.inp can not be found, please check the location.

ERROR: Lines to TOP level matching failed

This error indicates that there is a problem matching the data in levels.dat with what is found in TOPBase. This may indicate corrupted database files. Restore the original database files, and if the error still occurs, please contact the NEQAIR developers.

ERROR: NEQAIR no longer supports Gaunt factor input. TOPBase data required

This error indicates that NEQAIR did not find the TOPBase files in the database directory, and should have been preceded by a message indicating TOPBase files were not found. Check that the database directory contains the files e*XY.XY*, p*XY.XY* where *XY* is the atomic number of each atom for which b-f has been selected.

BFCONT requires an atom, its ion and electrons.

This error indicates that the bound-free option was selected with NEQAIR, however, not all of the following was found in LOS.dat: the atom, its ion and electrons, please check LOS.dat.

neqERROR: # of points in *xxx* exceeds MaxPoints constant. Increase MaxPoints to > *yyy* and recompile.

This error should not be displayed during normal usage of the code, and suggests that one of the TOPBase files has been changed from the distribution package. If this error does show up, please restore the p*XY.XY* files in the DATABASE directory. If the error persists, contact the NEQAIR developers.

ERROR: TOP state split over multiple QSS Levels

or

ERROR: Top Base level degen does not match LEVELS.dat degen

or

ERROR: QSS Term list does not match degeneracy

or

ERROR: *xxx* QSS Level j does not match LEVEL.dat degeneracies

These errors indicate that there was a problem matching the levels between TOPBase, QSS and LEVEL_ATOMS.dat. Restore the DATABASE files and if this error persists, contact the NEQAIR developers.

The # electronic diatomic band systems entered > MaxBands

or

The # IR diatomic band systems entered > MaxIRbands

Number of molecules in qssm calculation > MaxDiatom

or

 # dissociation cross-sections > MaxMolStates

or

'# electronic transitions > MaxMolTrans

or

No. of atomic systems entered exceeds MaxAtoms

This error message indicates that there are more bands/states/transitions requested in neqair.inp than it currently is setup to handle. Verify that extra items have not been added to neqair.inp. If this error continues to show up, please contact the NEQAIR developers.

Unable to open line-of-sight file LOS.dat.

This error indicates that NEQAIR cannot find the LOS.dat file that is needed for the calculation. Please check that LOS.dat is located in the current working directory.

Reorderions error: ions of species *xxx* are included but not the neutral atom or diatomic molecule

This error occurs if there are no atoms or diatomic molecules but there are atomic or diatomic ions. Check LOS.out to ensure each ion has a corresponding neutral.

BFCONT requires the ion for *xxx*

This error indicates that bound-free radiation has been selected for a certain species in neqair.inp, but the ionized state of the species is not included in LOS.dat (the ionized number density is required for this calculation): please double check LOS.dat, or turn off b-f for this atom.

Unable to open intensity.out

This error indicates that scan only was selected in neqair.inp, but the intensity.out file to be scanned was not found. Please check that intensity.out is located in the current working directory.

ffcont requires ion for species *xxx*

or

The ffcont calculation requires an atomic ion and electrons

This error indicates that free-free radiation has been selected for a certain species in neqair.inp, but the ionized state of the species is not included in LOS.dat (the ionized number density is required for this calculation): please double check LOS.dat.

Singular matrix in QSS; *xxx*

This error indicates that a unique solution to the QSS equations cannot be found. Verify the input files (LOS.dat) are correct.

Unable to open LEVELS_ATOMS.dat database file. Expected path name: *xxx*

or

Unable to open LINES_ATOMS.dat database file. Expected path name: *xxx*

or

Unable to open EXCITE_ATOMS.dat database file. Expected path name: *xxx*

or

Unable to open LEVELS_MOLE.dat database file. Expected path name: *xxx*

or

Unable to open LINES_MOLE.dat database file. Expected path name: *xxx*

or

Unable to open EXCITE_MOLE.dat database file. Expected path name: *xxx*

Please check that the DATABASE subdirectory is currently located in the path directory specified in neqair.inp. If this correct, please check that EXCITE_ATOMS.dat, LINES_ATOMS.dat, LEVELS_ATOM.dat, EXCITE_MOLE.dat, LINES_MOLE.dat, LEVELS_MOLE.dat are in the directory

Failed to find 1st repulsive quantum # for *xxx* electronic state *yyy* in *zzz* iterations
******* tol = *aaa*, xrepul =, *bbb* *******

This error should not be displayed during normal usage of the code. If this error does show up, please contact the NEQAIR developers.

QSS for *xxx* also requires atom and electron densities

This error indicates that the QSS option was selected with NEQAIR, however, the atoms comprising the named molecule and/or electrons were not found in LOS.dat. Please check LOS.dat.

Unable to open file CDSD_CO2.txt

This error indicates that the CO_2 IR band system was turned on, but could not find the file CDSD_CO2.txt. Please check the path directory in neqair.inp, and that this path points to the correct DATABASES directory in which CDSD_CO2.txt can be found.

Transition is forbidden. Only allowed transitions are permitted in this version of NEQAIR.

This error should not be displayed during normal usage of the code. If this error does show up, please contact the NEQAIR developers.

Unable to open neqair input file, neqair.inp

This error indicates that the neqair.inp file was not found. Please check that neqair.inp is located in the current working directory.

ERROR reading database path

This error indicates the DATABASES directory needed to run NEQAIR could not be found. Please check the directory path in neqair.inp

Error in LOS.dat, change in distance not positive at LOS point *x*

This indicates that there is either a negative or zero delta in distance at LOS point *x*. Please check that you have enough significant figures in distance to allow the delta to be positive.

Warning: QSS produced a non-physical result. QSS has not been run for NO at T = *x* K and Tv = *y* K

This warning indicates that the QSS solver could not calculate a physical result for the line of sight point corresponding to T = *x* and Tv = *y*. NEQAIR switched to using Boltzmann for this point. This warning usually only occurs for low temperature points ahead of the shock, and so the radiance calculated by switching to Boltzmann should be negligible for that point. However, if the QSS answer were to be used while QSS calculates a physically impossible answer, the result can be nonsensically high. The switch to Boltzmann occurs if the populations calculated by QSS are below zero.

[1]

[2] Rerdtyyg8