NEQAIR v15.0 Release Notes
Nonequilibrium and Equilibrium Radiative Transport and Spectra Program

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1 Acknowledgements and NEQAIR Version History

The current version of NEQAIR has been based upon the work of many others across approximately 24 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
NEQAIR2009 v1-v8	2009-2012	Palmer, Cruden
NEQAIR v13.1 - v13.2	2013	Cruden, Brandis
NEQAIR v14.0	2014 - 2015	Cruden, Brandis
NEQAIR v15.0	2016 - 2019	Cruden, Brandis

2 Introduction

NEQAIR v15.0 provides the first steps to improved coupling between NEQAIR and the DPLR CFD code, which will be fully realized in v15.1. The plan is to release NEQAIR v15.1 and DPLR 4.05 at the same time. The improvements implemented in NEQAIR v15.0 have focused on improving stability, solution robustness, usability and providing different options for running the code. It is also the first version of the code to have a new input file and line of sight format since 2009. Backward compatibility with previous formats of the input files (neqair.inp and LOS.dat) has also been provided. NEQAIR v15.0 supersedes the prerelease of this version, as well as NEQAIR v14.0, v13.2, v13.1 and the suite of NEQAIR2009 versions. These updates have predominantly been performed by Brett Cruden and Aaron Brandis from AMA Inc at NASA Ames Research Center between 2016 and 2018.

NEQAIR v15.0 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 v15.0, 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 or LAURA, and that lines of sight have been constructed and written out in the format required by NEQAIR v15.0.

There are two principal modes for running NEQAIR v15.0. In the first mode NEQAIR v15.0 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 v15.0 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 v15.0 uses 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). Atomic species that are currently present in the NEQAIR database include: N, O, C, H, He, Ar, Fe, Al, Cr, Cu, K, Mg, Na, Ni, S, Si. 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 and triatomic band systems in the NEQAIR database include:

- N_2 (1$^+$), (2$^+$), (Birge-Hopfield I), (Birge-Hopfield II), (Carroll-Yoshino), (Worley-Jenkins), (Lyman-Birge-Hopfield)
- N_2^+ (1$^-$), (A-X)
- O_2 (Schumann-Runge)
- NO (β), (γ), (δ), (ε), (β'), (γ'), (IR)
- CO (4$^+$), (IR)
- CN (violet), (red), (IR)
- C_2 (Swan)
- OH (A-X), (IR)
- H_2 (B-X), (C-X), (B'-X)
- MgO (B-X), (B-A)
- SiO (X-A), (A-E)
- CO_2 (IR)
- NH (IR)
- CH (IR)
- C_3

Band system parameters come from various sources including da Silva (da Silva, 2006), Bauschlicher (Bauschlicher, 2016 & 2017), Gilmore et al. (Gilmore, Laher, & Espy, 1992), Laux, C. (Laux, 1993) and Hyun and Park. (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.

A similar approach as used for CO_2 has been applied to C_3. C_3 can significantly absorb VUV/UV radiation. A line list was calculated by David Schwenke at NASA Ames Research Center. C_3 has been included in NEQAIR for the first time in V15.0.

NEQAIR computes bound-free continuum radiation between ionized atomic species and electrons using data from TOPBase (Cunto, Mendoza, Ochsenbein, & Zeippen, 1993 and Bautista, 1997). 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 Recent Updates to NEQAIR

- The mechanics of the QSS calculation have been substantially updated.
- New species are included in the NEQAIR database
- Write emission / absorption coefficients as output files
- Fast spectral grid
- Improved flexibility for specifying desired outputs
- Build and compile with gfortran in addition to intel (v14.0 compiled with intel, but had issues with gfortran)
- More robust to solve for a wider range of conditions, including different methods for solving the non-Boltzmann equations
- New neqair.inp LOS.dat input file formats
- Reduced memory usage
- Implementation of molecular non-local calculation
- Updated CO ground state constants in LEVELS_MOLE.dat
- Added first 4 states of CH to LEVELS_MOLE.dat
- New ability to write out excited state populations as output
- Added escape factor calculation for molecules
- Allow Blackbody boundary to be specified in shock tube mode
- Set a wavelength cutoff above which QSS treats bands as optically thin, if the region is not solved explicitly
- Fix 'out of bounds' error with Hydrogen level calculation
- Corrected some hang ups in non-Boltzmann solver
- Added logic to allow running Boltzmann and Saha for populations output
- Fixed error in CDSD memory allocation
- Corrected NO Frank Condon factors in EXCITE_MOL.dat
- Modified Non-Boltzmann to set untreated states in equilibrium with their nearest neighbor instead of the ground state. A similar change was made for the high energy (13, 14, 16) states of N_2. This reduces spurious atomic and molecular radiation observed in some cases.
- Franck Condon Factors in EXCITE_MOL.dat for NO beta, gamma, delta updated to be consistent with LINES_MOL.dat
- Added Spatial Convolution option for shock tube mode
- Updated some excitation rates in EXCITE_ATOMS.dat based on recent calculations by Huo.
- Updated excitation database for N_2. In particular, the $C^3\Pi$ state is now calculated by non-Boltzmann, which controls N_2 2nd Positive Emission
- New output file, coupling.out. Contains data that can be used with CFD coupling calculations.
- Add heavy particle excitation to atomic non-Boltzmann
- Removed normalization of atomic electron impact rates
- Added Stark broadening parameters for Hydrogen

5   Overall Structure of NEQAIR

The organizational structure of NEQAIR was significantly streamlined in the 2009-2013 timeframe, and now updated again for v15.0. The main subroutine structure is as follows:

```
program neqair

    call SetUpParallel

    call readLOS

        call readSpeciesNames

        call reorder_species

    call read_neqair_input

        call MPI_BCAST

    call computeRadiation

       call setupGrid

           call compute_spectral_grid

       call calcEmisAbs

           call computeSpeciesRadiation

               call atomic_radiation

               call molecular_radiation

       call computeThin

       call precomputeIntensity

       call computeIrradiance

           call setupIntegration

           call wallHeating

       function integrateSpectralIntensity

       call computeNormalLOS

           call setupIntegration

           call computeLOS

    call MPI_Finalize
```

6   Compiling the Code

There is a build script that is sent along with the NEQAIR distribution package. It is recommended to compile the code using ifort and mpif90. For the local cluster in the TSA division at NASA Ames Research Center, we are using ifort version 16.0.2.181 (some issues with the code have been identified when compiled with version 18.0.1.163) and

Open MPI version 3.0.0. The default build script distributed with the code should be able to install NEQAIR. The module load commands listed in the build script will need to be updated to follow the nomenclature of your cluster system. The code has also been compiled with GNU gcc 7.3.0. v14.0 was unable to compile with gfortran, so this provides increased flexibility for v15.0. On the NAS Pleiades cluster, ifort version 2018.3.222 and SGI's MPI version mpt 2.17r13 have been used. 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. 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.

7   User Interface Updates

Although the NEQAIR input file has been updated, NEQAIR v15.0 should be backward compatible with input files from NEQAIR v14.0 (and likely with older versions, such as the 2009 versions of the code). Furthermore, converters to update the new format are provided for both neqair.inp and LOS.dat.

8   Guide to NEQAIR Input Files
This section will run through the options available, and the files needed to run NEQAIR v15.0.

8.1   Overview of Required NEQAIR Data
For each line of sight point in the flow field, NEQAIR requires the distance along the line of sight, 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.

Intensity.in can be used to apply a defined spectral radiance at the first line of sight point.

Emissivity.in can be used to apply emissivity/reflectivity at the final point in the line of sight, e.g. optical property of the TPS

LOS 1   LOS 2   LOS 3   ...   LOS n
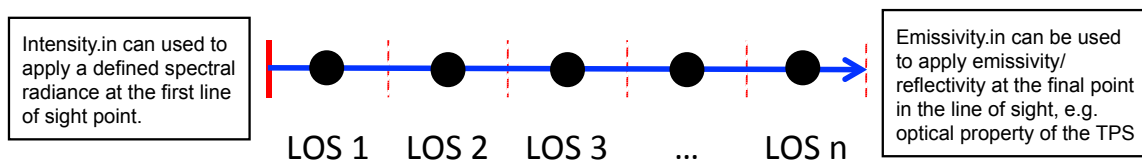
Figure 1. Diagram of basic line of sight for NEQAIR.

8.2   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 neqair > neqair.out`"). NEQAIR also requires two other files, neqair.inp and LOS.dat. These files are described in the following sections.

8.3   run_neqair.pbs

PBS script:

```
#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 intel/18.0.1.163
module load openmpi3/3.0.0

module load neqair/15.0

# Run the program
mpiexec neqair > neqair.out

# Report when the job finished
date
```

Slurm script:

```
#!/bin/bash
#SBATCH --time=00:05:00
#SBATCH -n 72
#SBATCH --job-name="fire2"
#SBATCH --partition=batch

ulimit -s unlimited

rm -fr neqair.out

# Report when the job started
date

module purge
module load neqair/15.0

# Run the program
time mpiexec neqair > neqair.out

# Report when the job finished
date
```

The run file has been updated to account for the parallelization of NEQAIR in v15.0 (parallelization originally implemented in v14.0). The number of nodes requested for the job is stated with the ppn variable. This is specified in the line:

```
#PBS -l nodes=3:ppn=24 or #SBATCH -n 72
```

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. Shock tube mode is an exception to this.). 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 or #SBATCH --time=00:05:00
```

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

```
#PBS -N fire2  or #SBATCH --job-name="fire2"
```

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

```
#PBS -q batch  or #SBATCH --partition=batch
```

This line selects the queue for the job on the cluster. Here 'batch' is used in the example.

NEQAIR is executed with the following line:

```
# Run the program
```

```
mpiexec neqair > neqair.out
```

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

```
neqair > neqair.out
```

8.4 neqair.inp:

In past versions of NEQAIR, inputs were selected by marking the appropriate location in neqair.inp with an 'X'. However, with v15.0, a string of characters is used to select what style of calculation is desired, and what outputs the user wants.

```
15.0
***************************
NEQAIR Input File Template
For versions newer than 14.0, the version number is listed on the first line
The inputs are separated below, each section enclosed by ----'s
The first line in the section is a description
The second line is read by NEQAIR as a character sequence
In some cases additional lines may follow
A blank line ends the input section
Following lines are used for comments and ignored by the code
***************************
Line 0: Header - anything between here and the ---'s writes to stdout
aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa <- 1st format line
-------------------------
```

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 "*********…"

```
Line 1: Database path - if empty, looks for local DATABASES directory
/apps/pkgs/neqair/intel/openmpi3/15.0/DATABASES
-------------------------
```

This specifies the location of the code's DATABASE files. The above is the DATABASE location maintained on cedar. This line may be left blank if the DATABASES folder is in the working directory.

```
Line 2: Output type : a string of letters indicating one or more output files
LMS

Allowed input choices for line 2:
(I)ntensity.out - write intensity vs. wavelength (high resolution)
Intensity_(S)canned.out - write the scanned intensity v. wavelength file
(L)OS.out - write radiance versus position on the normal line of sight
(R)adiance only output
(H)eat flux only output
(P)opulation - write state population for each atom at each LOS point
(A)bsorbance/Emittance - write absorbance/emittance at each LOS point
(C)oupling.out - data needed for flowfield/radiation coupling
(2) a 2 following an I or S means the output is in columns, where each column is
an LOS point
(M) write general messages to stdout
```

The request for output in v15.0 has been significantly simplified. Just type the string of letters corresponding to that output that you require.

- (I)ntensity.out: the largest output file which contains the unconvolved high-resolution spectra.
- (L)OS.out: write radiance versus position with a breakdown by the wavelength ranges specified in the input file.
- (R)adiance only output would mostly be used when running full angular integration (3-D ray tracing) calculations where the radiance result is required, with no other output files. Note that Radiance output is written by default for certain geometry options.
- (H)eat flux only output is for when only the final heat flux value is required. Note that Heat Flux is written by default for certain geometry options.
- (P)opulation writes the state populations for each atom in the calculation for each point in the line of sight.
- (A)bsorbance/Emittance writes out the absorbance and emittance as a function of wavelength.
- (C)oupling.out provides the derivative of heat flux needed to couple with a CFD code's energy balance.
- (2) following an I or an S, means that the intensity or intensity_scanned file is reported in two dimensions, as a function of wavelength and distance. N.B. The 2-D intensity.out file can be quite large (several GB), so this combination should only be selected if really necessary.

```
Line 3: State population method
N Q L 1.0

Allowed input for Line 3:
(B) Boltzmann
(N) Non-Boltzmann followed by (optionally) non-boltzmann method and (required)
absorption method.
    Valid choices for method are:
        (Q) Traditional QSS (adjusts ground state)
        (T) Time derivative limited (adjusts slowest eigenvalue)
        (R) Reaction  residual  limited  (adds  a  reaction  rate  proportional  to
Boltzmann distribution)
        (F) Flux limited (adds a term accounting for convection - most stable,
recommended, default)
    Valid choices for absorption method include:
        (L) Local Escape factor approximation, followed by a float for d
        (C) Constant escape factor, followed by the value
        (N) Non-local radiation/QSS coupling
(S) Saha (atoms only)
(F) Input from File (file names pop-xxx-xxx)
(A)  Do  not  calculate  state  populations,  instead  read  absorption/emission
coefficients from files
      ae.nnn.  The order in which to process the nnn files is obtained from
LOS.dat
If different settings are desired for molecules and atoms, include a second line
for molecules


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

This line specifies how to calculate the excited state populations in the radiance calculation, or to bypass the state population calculation entirely by providing additional input files. In general, states may be calculated as a Boltzmann distribution, as the solution to non-Boltzmann conservation equations (formerly referred to as QSS), or by the Saha equation. Not all of these options are available for all species. Figure 2 shows an example of the different excited state populations.
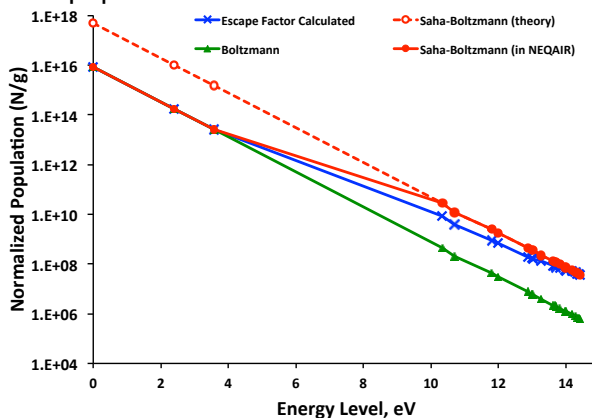
Figure 2. Various populations available in NEQAIR

In non-Boltzmann mode, there are several options for how to solve the QSS equations. The options described above include the traditional QSS from previous NEQAIR versions ('Q') and three new options ('T', 'R', 'F') where 'F' should be considered the new default. If you come across a case where the simulation fails, trying an alternate QSS method is recommended. This option may be omitted, in which case 'F' is used by default. The next input specifies the methodology for determining the escape factor. The most common approach is the "local" approximation which requires a characteristic distance in cm.

Typically a value of 1.0 cm is used, and would be entered as L 1.0. Generally, this number should be the same order of magnitude as the shock-standoff distance. Alternatively, a constant escape factor can be specified (e.g. C 0.0) or running the more accurate, yet more computationally expensive, non-local method (e.g. N). This method iterates on the radiation calculation in both directions, so does not require an approximation for escape factor. If the excited state populations and/or absorption/emission coefficients have been calculated external to the NEQAIR simulation, the option 'F' or 'A' can be specified, respectively. If 'F' is selected, NEQAIR will use the specified populations to calculation the emission/absorption coefficients and perform the radiative transfer calculations. For, 'A', the absorption/emission coefficients are read from files and hence radiative transfer calculations will be performed. Note that 'A' or 'F' may also be specified in conjunction with a non-local calculation to set a starting point for the iterative procedure. (Otherwise, the starting point is a standard non-Boltzmann solution with local escape factor)

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. If the NonLocal method is selected, NEQAIR will iteratively calculate the level of excitation through the line-of-sight for atomic radiation, and therefore an escape factor is not used, see Figure 3. 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. The NonLocal answer should be more precise, 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, intensity.out and intensity_scanned.out should not be specified as outputs. 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 final point is treated according to the emissivity selection.
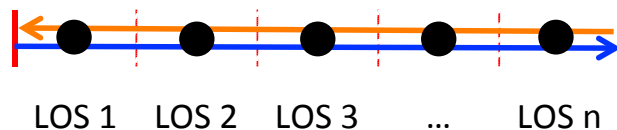

LOS 1   LOS 2   LOS 3   ...   LOS n
Figure 3. Two way radiative heat flux.

.

```
Line 4: Geometry
T

Allowed input for Line 4:
(T) Tangent Slab - calculate tangent slab heat flux
(C) Spherical Cap - follow with two floats for Rnose and Shock Div
(S) Shock Tube - follow with a float for tube diameter
(L) Line of Sight - calculate radiance on line
(B) Blackbody function (follow with float for temperature, otherwise uses Tt at
first LOS point)
(P) Calculate Populations only (requires P output, Line 2)
(X) Perform scan on existing intensity.out (S must be selected on Line 2)

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

This section defines the geometry, and thus the type of calculation NEQAIR is to perform. 'T' is the most common mode for NEQAIR to be run, which calculates the spectral radiance and the wall-directed heat flux, see Figure 4a. If Line-of-Sight is selected ('L'), NEQAIR will calculate the spectral radiance and wall directed radiance, see Figure 4b. This option is useful for 3-D full angular integration calculations, where the tangent slab method is not desired. If Shock Tube, 'S', is selected, the radiance will be calculated perpendicular to the line of sight, using a constant slab of width specified after 'S' (typically this would be the shock tube diameter), see Figure 4c. 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.

If the Spherical cap model is used, see Figure 4d, 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].

Bow Shock

Discrete Line of Sight points

Body

Stagnation Point

θ

Shock layer

(a) Tangent Slab

Discrete Line of Sight points

Body

Bow Shock

Line of Sight

Shock layer

(b) Line of Sight

Discrete Line of Sight points

Shock

d
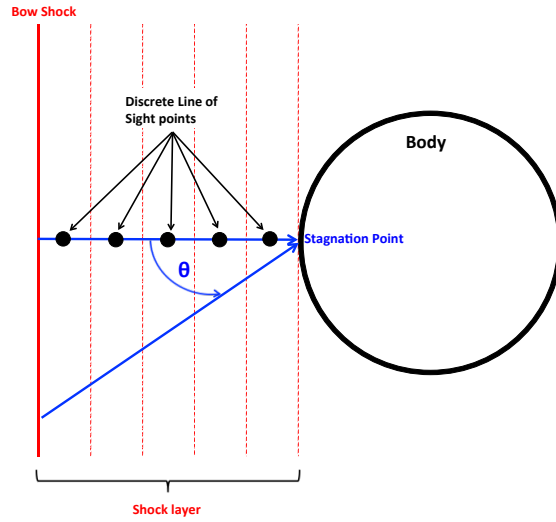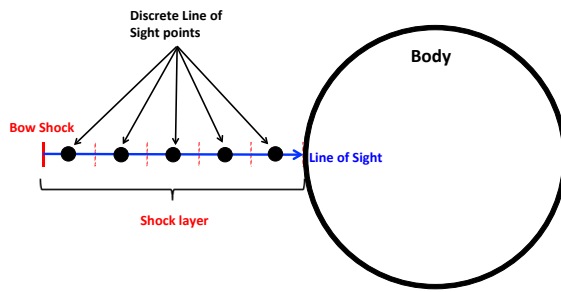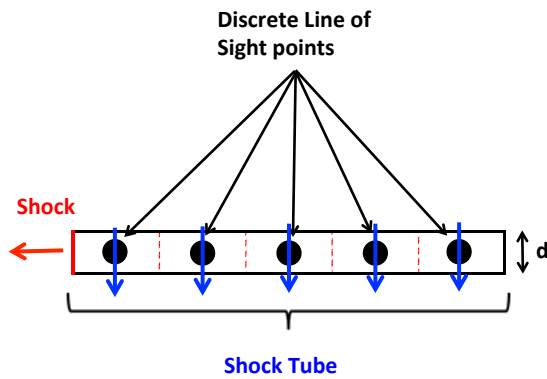
Shock Tube

(c) Shock Tube
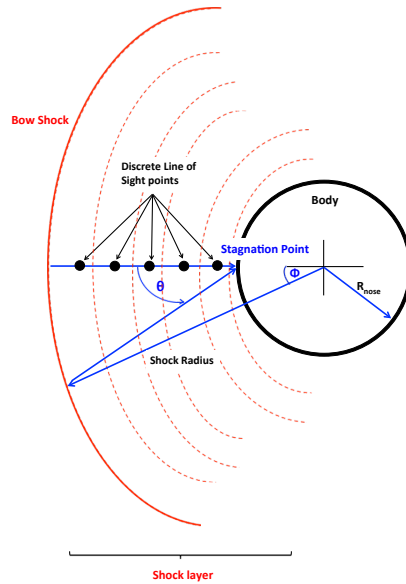
(d) Spherical Cap
Figure 4. Different geometry options available in NEQAIR.

The Blackbody calculation, 'B', if selected, calculates the black body radiance at the specified temperature. If no temperature is provided after 'B', NEQAIR will use T_t from the first LOS point. If 'P' is selected, NEQAIR will calculate the populations of the all the species, but does not calculate the emission/absorption spectra or radiative transfer. This option can also be useful to see what format NEQAIR expects the populations input to be (Note: requires P output on Line 2). If 'X' is selected, NEQAIR will perform a spectral scan on a provided high resolution intensity.out file (Note: requires S output on Line 2).

```
Line 5: Boundary Conditions
N
B

First line is boundary at LOS point 0. Options are:
(B) Blackbody
(I) read Intensity.in
(N) no initial radiance

Second line is boundary at final LOS point
(I) read emissivity.in
(G) Greybody, follow with Emittance/Absorbance (0-1.0) and Transmittance (0-1.0)
(B) Blackbody (at final LOS point temperature)
Note this boundary condition is used to convert data into an absorbed heat
flux/radiance
Use 'B' if only the incident radiance/flux is desired
This value does however, materially affect the calculation for Non-local
populations

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

This section specifies the boundary conditions for the calculation. The first line provides the boundary condition for the free stream side of the line of sight (first LOS point). The second line provides the boundary condition for the end/wall side of the line of the sight (last LOS point).

For the first LOS point, the options are for no initial radiance ('N'), which would be the most common value used. Alternatively, an initial radiance can be specified with a black body radiance or with file detailing the initial intensity (intensity.in, see section 8.6.1)

For the last LOS point, the options are for black body radiance at the temperature of the last LOS point ('B'), which would be the most common value used. Alternatively, an emissivity can be specified by a grey body through Emittance/Absorbance (0-1.0) and Transmittance (0-1.0) or with file detailing the emissivity (emissivity.in, see section 8.6.2)

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.

Some relevant definitions:

emissivity: the relative ability of the 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.

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

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.

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

```
Line 6: Bands
I N2 BH2 LBH BH1 WJ CY
NO del eps bp gp IR

Allowed input:
(A) Include all bands/features that match species list
(O) Omit selected bands or features
(I) Include only selected bands or features

If (O) or (I) is selected, follow with the following (optionally on separate
lines):
N, O, C, H, He, Ar, Fe, Al, Cr, Cu, K, Mg, Na, Ni, S, Si - available atoms
N2, N2+, NO, O2, CN, CO, C2, H2, NH, CH, CO2, C3, MgO, SiO - available molecules

For atoms, can optionally follow with bf,bb, and/or ff
For molecules, the following band choices can be included
N2 - 1+, 2+, BH2, LBH, BH1, WJ, CY
NO - beta, gam, del, eps, bp, gp, IR
CN - VIO, RED, IR
H2 - B-X, C-X, B'-X
CO - 4+, IR
OH - A-X, IR
MgO - B-X, B-A
SiO - X-A, A-E

Specific vibrational modes can be (de)selected by following the band name with
(XXX,YYY) where XXX and YYY are specifiers of upper and lower vibrational modes,
respectively
These may be a single number or a range of numbers (separated with a dash, e.g.
0-12)
To specify all possible vibrational levels, use an 'X' or negative number (e.g.
"(0-5,X)")
Multiple vibrational selections may be specified per band by writing them in
sequence

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

This section details what species transitions and bands are included in the NEQAIR calculation. If 'A' is selected, NEQAIR will run all transitions and bands corresponding to the species included in LOS.dat. Alternatively, 'I' or 'O' can be selected to specify individual species or omit species, respectively. If 'I' is selected, you can run just CN as example, by typing "I CN". If you want to run all bands, except CN, you can type "O CN". Furthermore, bound free (bf), bound bound (bb) and free free (ff) transitions can be specified for atoms and different band systems can be specified for molecules. Specific vibrational modes can also be selected or de-selected by following the band name with a vibrational transition (e.g. (1,1)) or range of transitions (e.g. (0-5,X)). The latter example indicates that transitions from upper levels from v'=0 to 5 and any lower level (denoted as 'X') be included. In the example above, N_2 and NO are activated, with the specific bands turned on for N_2: First positive (1^+), Second positive (2^+), Birge-Hopfield II (BH2), Lyman-Birge-Hopfield (LBH), Birge-Hopfield I (BH1), Worley-Jenkins (WJ) and Carroll-Yoshino (CY), and for NO: Delta (del), epsilon (eps), beta prime (bp), gamma prime (gp), Infra-Red (IR).

```
Line 7: Regions
855.5 2000 A 10 R 600
2000  6350 M 0.003 R 50
6350 16000 F 5 R 50

A series of lines specifying the region parameters.  This includes:
w1 w2 A/M n Rdd
w1, w2 are wavelength range in Angstrom
A/M/F is (A)uto,(M)anual or (F)ast Grid Spacing.  This is followed by n,
which is:
Grid Spacing (Angstroms) for Manual or
Points per Line for Auto and Fast
The next parameter is an optional "Range", with dd being the range value

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

For each region, a start and end wavelength, w1 and w2, must be defined in Angstroms. Note that NEQAIR expects the regions to be in order and continuous. Additionally, radiance calculated in one region is not broadened accurately into adjacent regions, so that the region boundaries should be chosen to lie in areas of the spectrum without significant features. If the grid spacing setting is set to 'A' ('A' for automatic, previously grid_type 1), the minimum spacing required for each region to resolve the thinnest linewidth is calculated by NEQAIR, based on the properties of the 2nd LOS point. In this case, points per line specifies the minimum number of grid points to use for each line (typically equal to 10, or 5 for fast mode.). If the grid spacing setting is set to 'M' ('M' for manual, previously grid_type 0), the grid spacing value specified by the user is used for that region. The automatic grid option can over-resolve the grid spacing required for an accurate answer, so running with an appropriately spaced manual grid can be significantly more efficient if running many cases. If the grid spacing is set to 'F' ('F' for fast), NEQAIR will calculate a grid spacing based on the mean linewidth for each region (as opposed to the minimum with 'A') in order to reduce the spectral grid size, and thus reduce the calculation time. Running in fast mode typically reduces run time with errors in heat flux on the order of less than 3%, but this not guaranteed for all classes of problems. If running in fast mode, it is suggested to not request intensity.out or intensity_scanned.out as output files to reduce computational time and as certain low radiance features may not be adequately resolved spectrally. '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. In the above example there are three wavelength regions specified. Region 1 is from 855.5 to 2000 Angstroms, using an automatic grid ('A') with '10' points per spectral line, and a range of ('600'). Region 2 is from 2000 to 6350 Angstroms, using a manual grid ('M') with a spectral spacing of 0.003 Angstroms, and a range of ('50'). Region 3 is from 6350 to 16000 Angstroms, using a fast grid ('F') with '5' points per spectral line, and a range of ('50'). Using 5 points per spectral line is suggested when running in Fast mode to further reduce computational time.

```
Line 8 : Scan (Only required if S selected on Line2)
0.1 Voigt 6.0 0.0

Which follows the format:
Sp Type Param-list
where Sp is the line spacing (float)
Type is the scan type (ICCD1, ICCD2, Voigt, SGauss)
Param-list is a list of scan parameterizations, generally is 2 or 3 float values

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 and may only be given on the Parameters Line
      Input parameters are Gaussian and Smearing components (in A)
---------------------------
```

This section describes the spectral scanning of the calculated spectral intensity. This output is obtained if 'S' is selected in Line 2, Output type. The results in intensity_scanned.out will be the spectrally scanned data from intensity.out (high resolution) using 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 be defined globally, by specifying a single slit function, or defined for each spectral region by listing multiple slit functions on separate lines. The Spectral Interval (spacing between scan points) needs to be defined in terms of Angstroms. Each spectral region then needs the lineshape's required input parameters along with an optional range value.

```
Line 9 : Spatial Scan (Optional - ShockTube mode only)
tri 1.0
ICCD1 1.0 0.1
1.0

Which follows the format:
Spatial Scan is the convolution of 3 functions, each specified on consecutive
lines
1st line: Optical Function (trap)ezoid or (tri)angular, followed by one or two
floats specifying base widths
2nd line: CCD Function: Same options as Scan (Line 8)
3rd line: Temporal Function: Treated as a square, float specifies widths

If this line is present, LOS.out will be the convolution of the true result
with this function
If this line is missing, LOS.out will not be convolved

To use a different SRF for each region, repeat these 3 lines N times
```

The last section describes the spatial scanning of the calculated intensity, only used when running in shock tube mode. This output is ignored if 'S' is not selected on Line 4,

Geometry. The data found in LOS.out and/or 2D intensity_scanned.out/intensity.out will be convolved with the spatial scan specified. The spatial scan contains three broadening components which are convolved with each other, as described above. The dimensions of the entries are in cm. The spatial function can either globally be defined by entering one group of three lines, or may be defined for each spectral region by entering three lines for each region. NEQAIR will stop reading the input file once a blank line is encountered, hence no blank lines should be inserted between regions. However, if it is not desired to broaden a shock tube solution, a blank line may be entered at the beginning of this section and the broadening functions will not be read.

8.5   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. For shock-to-body calculations, it is advisable that the first LOS point have a vibrational temperature of at least 500 K. There is a new version of the LOS.dat file for v15.0, which contains a header detailing the relevant information, followed by column separated data. Note, there are fewer significant figures in the below example for clarity of showing the format. The old-style formatted input file from v14.0 (and other older versions) will still work with v15.0

```
#15.0
#              This is the NEQAIR15 LOS.dat file
#
# An unlimited number of comment lines is allowed here
# The first line to begin with a numeric is the start of the LOS data
# This data is in row/column format, separated by white space
# The final text line contains the headers for the columns
#
# Valid entries for headers include:
#  n    - index of LOS number (optional)
#  x    - Distance on line of sight (cm).  May also be denoted as 'y' or 'z'
#  ntot - total number density (1/cm3, optional), if omitted, species densities are summed to get total
#  T    - Temperature (K).  Up to 5 different temperatures may (optionally) be specified:
#  Tt   - Translational Temperature (K).  Assumed same as T.  If omitted, set to Tr
#  Tr   - Rotational Temperature (K).  If omitted, set to (in order of preference) Tt, Tv, Te, Tel
#  Tv   - Vibrational Temperature (K).  If omitted, set to (in order of preference) Te, Tel, Tr, Tt
#  Te   - Electronic Temperature (K).  If omitted, set to (in order of preference) Tel, Tv, Tr, Tt
#  Tel  - Electron Temperature (K).  If omitted, set to (in order of preference) Te, Tv, Tr, Tt
#         (Tel currently not supported.  May be entered, but is not used in computation.)
#  XXX  - Any entry following these are assumed to be species names and densities (1/cm3)
#
  n       x       ntot        Tt        Tr        Tv        Te        CO2         CO         N2          O2
  1  0.00E+00  0.263E+17    4594.7    4594.7    2596.2    2596.2  1.066E+16  7.246E+15  7.260E+14  1.291E+14
  2  0.65E+00  0.198E+18    7997.6    7997.6    7811.0    7811.0  4.330E+15  9.026E+16  2.291E+15  3.198E+14


.
.
.

59  0.23E+02  0.104E+19    2002.3    2002.3    2002.3    2002.3  9.959E+17  2.904E+08  4.693E+16  5.101E+07
```

8.6   Optional Input Files

8.6.1   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.

8.6.2   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).

8.6.3   Populations Files

NEQAIR v15.0 can also accept state populations for all species along a line of sight as input. The naming convention for the file is: pop*xxx-y*.dat, where *xxx* is the LOS number, e.g. 002, *y* is the species name, e.g. N. An example file name would be pop002-N.dat. It is recommended that a calculation in NEQAIR be run with populations output in order to generate the file format which the user can then edit to reflect desired input. The file format for the population files is given below, and lists the energy level of the species, (normalized) population, and degeneracy. For atoms, the population density is normalized for convenience of providing and reading a Boltzmann plot. For molecules, however, the normalization factors are functions of temperature, and are not in general known by the user. Hence, for molecules the populations are not normalized. For the purposes of input, the first and third column of the population file are not used and only the second column enters the calculation. It is necessary to use the same levels, in the same order, as they occur in the population output files. This is the same ordering in the LEVELS_ATOMS.dat and LEVELS_MOLE.dat DATABASE files. Population output files also contain population information about ions and/or dissociation products. This data is ignored on population input files, and thus may be omitted if desired.

```
#     Energy Level      Normalized Population    Degeneracy
#        (1/cm)            (N/g), (cm^-3)            (g)
      0.000000E+00     1.890847228527914E+11        4.0
      1.922446E+04     1.461034317181443E+08        6.0
      1.923318E+04     9.550353545910858E+07        4.0
      2.883892E+04     5.332842128761898E+06        2.0
      2.883931E+04     1.065638633436139E+07        4.0
      8.328407E+04     6.797628860955761E+02        2.0
      8.331783E+04     1.259679740342129E+03        4.0
      8.336462E+04     1.699958424305023E+03        6.0
      8.613735E+04     1.077832002045441E+00        2.0
      8.622051E+04     1.786403579345035E+00        4.0
      8.810726E+04     3.772946286436007E-02        6.0
      8.815117E+04     2.277730227729946E-02        4.0
      8.817057E+04     1.090023515279256E-02        2.0
      9.358155E+04     7.685144256795453E+02        2.0
      9.477088E+04     5.231321178159321E+01        2.0
      9.479349E+04     9.941573244908969E+01        4.0
      9.483089E+04     1.370399820238590E+02        6.0
      9.488182E+04     1.628585314002765E+02        8.0
      9.547531E+04     1.065082336330203E+01        2.0
      9.549369E+04     2.043514103918846E+01        4.0
      9.553215E+04     2.810151159693128E+01        6.0
      9.675084E+04     1.193405463617921E+00        4.0
      9.678768E+04     1.098091283430900E+00        4.0
      9.686405E+04     1.386088503897164E+00        6.0
      9.777018E+04     5.963779610276271E-02        2.0
      9.780584E+04     1.100423583684138E-01        4.0
```

8.6.4 Absorption/Emission Coefficient Files

NEQAIR v15.0 can optionally accept absorption and emission coefficients as input at each line of sight point. The naming convention for the file is: ae.n, where *n* is the LOS number. This file is formatted in three columns, containing wavelength (in A), emission coefficient (in W/cm^3-sr-um) and absorption coefficient (in cm^{-1}). Non-numeric text at the beginning of these files will be treated as headers and ignored. The wavelengths need not be equispaced or follow the spacing of the wavelength grid – data will be interpolated onto new grids by NEQAIR. Wavelength regions are set as specified in neqair.inp. The grid spacing will follow neqair.inp (for manual grid) or the minimum spacing in the file for that region (for automatic grid). When the absorption/emission coefficients are read, the only information from LOS.dat that is used is the LOS number, which identifies the order in which to process the files, and the distance, which sets the spacing between points. This is not the case for non-local simulations, however, where these files are used to "restart" the iterative solver. A sample format for these files may be obtained by running NEQAIR with the 'A' option on Line 2.

9   Guide to NEQAIR Output Files

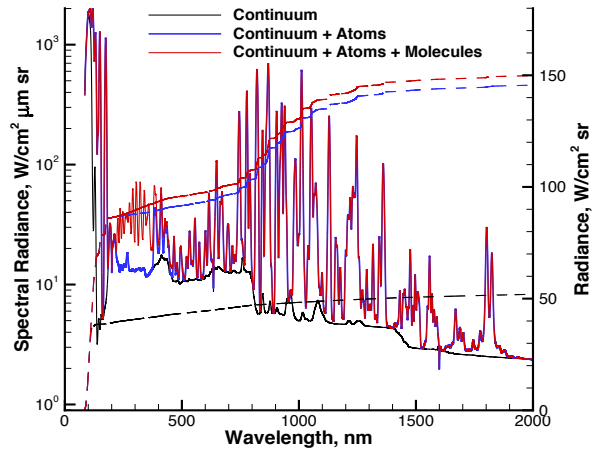## 9.1 Various Mechanisms Identified in Output

Figure 5. Different components of spectral radiance.

9.2 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 high resolution comparison of two computed spectra. An example of this output is shown in Figure 6.
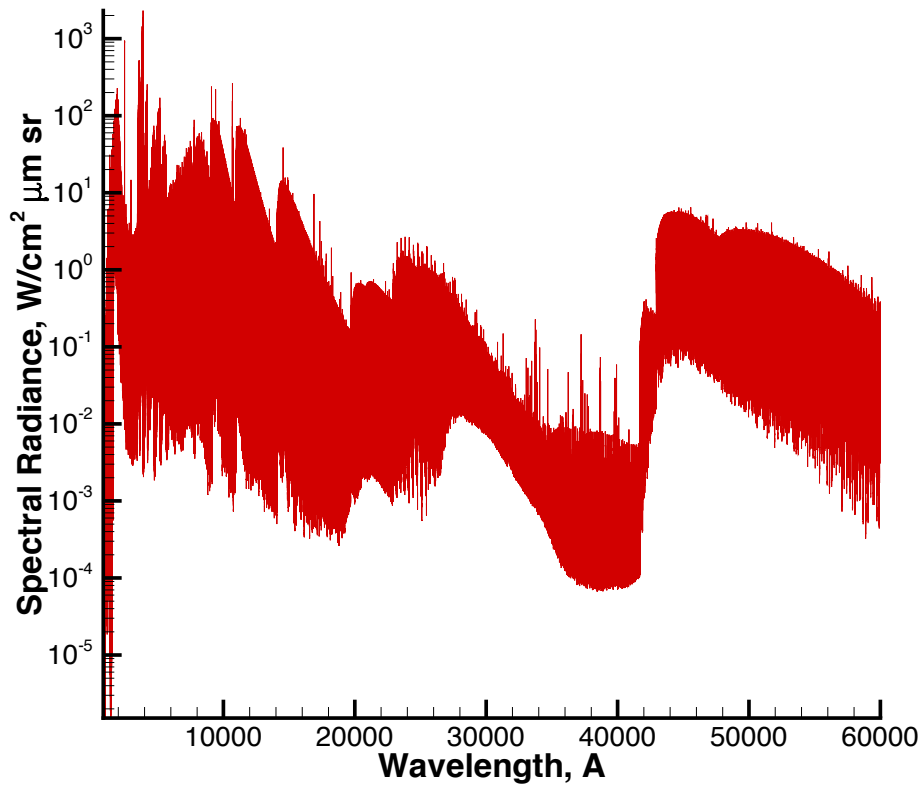
Figure 6. intensity.out for the NEQAIR Mars test case.

9.3 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. An example of a 2D intensity_scanned.out is shown in Figure 8.
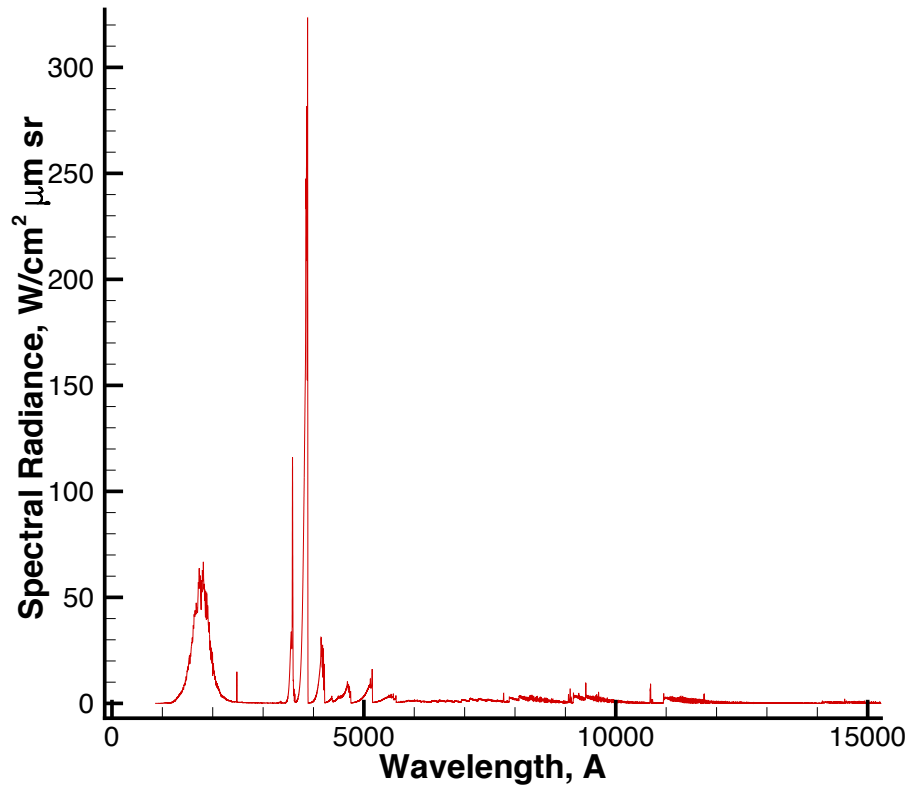
Figure 7. intensity_scanned.out for the NEQAIR Mars test case.
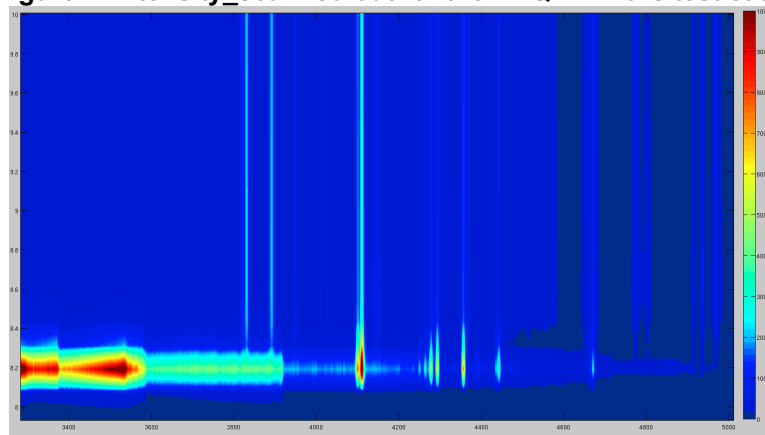
Figure 8. 2-D intensity_scanned.out for high speed Earth entry

9.4 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 in radiance or heat flux mode and Figure 10 in shock tube mode.

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).
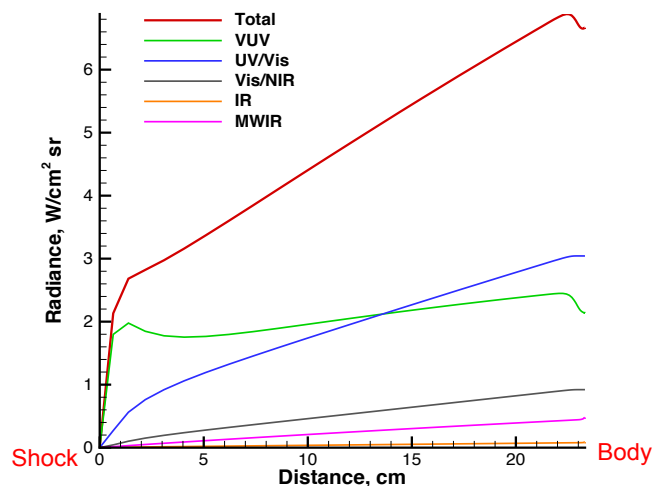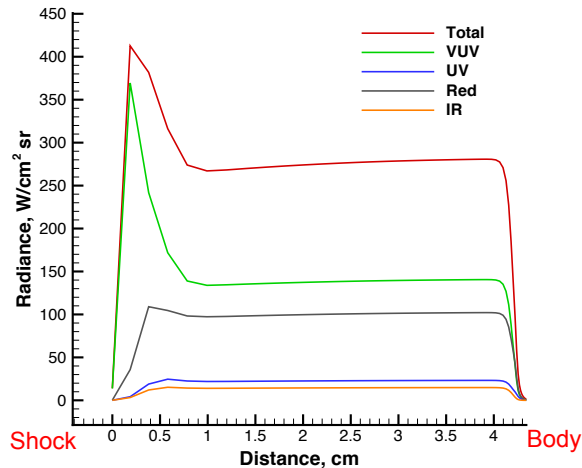
9.5 Populations output

As well as being an input (described in Section 8.6.3), populations can be an output as well. These files give you the state populations for each species at each point in the line of sight as calculated by NEQAIR. It is recommended to run the output option first, even when you want to use populations as input, to understand the exact format and data NEQAIR is expecting as input. The population files contain all the information required to produce a Boltzmann plot. Energies are in the first column. Populations in the second column are normalized for atoms and un-normalized for molecules. Normalization factors are given in the third column. These factors may be used to produce Boltzmann plots for molecules or recover the absolute state density for atomic levels.

9.6 Absorption/Emission Coefficient output

As described under input in Section 8.6.4, the absorption and emission coefficients can be an output as well. These may be useful for doing very detailed examination of a solution or finding the absorbance at a particular point (say, for absorption spectroscopy). Alternatively, the files may be used to "restart" a non-local solution or to re-order one or

more lines of sight that have already been solved. These output files are not equispaced in wavelength – to reduce filesize and disk write time, the solution is downsampled to remove points that can be found by linear interpolation.

9.7   Coupling.out

NEQAIR can generate an output file that contains information necessary to perform a coupled radiation/CFD solution. This includes the energy lost to radiation at the LOS pt. in W/cm^3, sometimes referred to as the "radiation source term" or "divergence of radiative flux" and the rate of some photo-driven reactions, in cm^{-3}-s^{-1}. The former would typically be removed from the total and electronic energy equations in the flow solver, while the latter would added/removed from the appropriate species conservation equations, should the solver make such allowances.

9.8   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 'M' is selected on Line 2 (as is in the example given below), the file gives information regarding the neqair run, e.g. what parameters and radiating transitions were included. If only the heat flux or radiance is required, specify 'H' while in Tangent Slab mode or 'R' while in Line of Sight mode, respectively. To get both radiance and heat flux, you can specify HR while in Tangent Slab mode.

```
                        STANDARD OUTPUT FOR NEQAIR


        Run Type:  Heating (Stag Pt.) Calculation
        Geometry:  Tangent Slab
        State Populations are calculated by flux limited Non-Boltzmann for Atoms and
Molecules
            Local approximation with self-absorption only is applied with d =  1.00 cm
        Database file path =
/home4/tsa/apps/neqair/15.0/intel/2018.3.222/mpt/2.17r13/DATABASES/
        Outputs : General messages will be written to stdout
            Heat Flux will be written to stdout
            The scanned line of sight radiance will be written to intensity_scanned.out
            The radiance accumulated along the line of sight will be written to LOS.out
            The stagnation point heat flux will be written to stdout
        Boundaries:  Initial radiance is zero
                    Final boundary is a blackbody


                        Spectral Systems and Parameters


                            Atomic Systems


        Atom          b-b            b-f            f-f
    1  C              T              T              T
    2  N              T              T              T
    3  O              T              T              T


            Molecular Band Systems


     1  CO 4+    (0-17, 0-20)
     2  CO IR    (1-38, 0-35)
     3  N2 1+    (0-15, 0-15)
     4  N2 2+    (0-4, 0-15)
     5  N2 BH2   (0-15, 0-13)
     6  N2 LBH   (0-15, 0-13)
     7  N2 BH1   (0-15, 0-13)
     8  N2 WJ    (0-4, 0-13)
     9  N2 CY    (0-8, 0-11)
    10  O2 SR    (0-12, 0-21)
    11  NO beta  (0-15, 0-21)
    12  NO gam   (0-8, 0-22)
    13  NO del   (0-7, 0-22)
    14  NO eps   (0-5, 0-22)
    15  NO bp    (0-7, 0-20)
    16  NO gp    (0-4, 0-14)
    17  NO IR    (1-28, 0-25)
    18  CN VIO   (0-9, 0-9)
    19  CN RED   (0-9, 0-9)
    20  CN IR    (1-27, 0-24)
    21  C2 SWAN  (0-9, 0-9)
    22  CO2
```

```
        Wavelength Regions:

 region    w1        w2       range grid_type deltaLam  nPointsPerLine

    1    855.50   2000.00     600      A       N/A       10
    2   2000.00   6350.00      50      A       N/A       10
    3   6350.00  16000.00      50      A       N/A       10
    4  16000.00  39600.00      25      A       N/A       10
    5  39600.00 200000.00      25      A       N/A       10


--------------------------------------------------------------------------


Region 1 number of equispaced grid points =        825568
Region 2 number of equispaced grid points =       1315705
Region 3 number of equispaced grid points =        935314
Region 4 number of equispaced grid points =        837191
Region 5 number of equispaced grid points =       2086138


Radiative heating from    855.50 to   2000.00 angstroms =  5.204954E+00 W/cm2
Radiative heating from   2000.00 to   6350.00 angstroms =  1.669560E+01 W/cm2
Radiative heating from   6350.00 to  16000.00 angstroms =  5.403026E+00 W/cm2
Radiative heating from  16000.00 to  39600.00 angstroms =  5.199339E-01 W/cm2
Radiative heating from  39600.00 to 200000.00 angstroms =  2.483079E+00 W/cm2


Total radiative heating from    855.50 to 200000.00 angstroms =    30.30659 W/cm2
```

10 Utilities to Update Old Formatted Input Files

10.1 Convert LOS.dat to v15 format

There is a utility released with NEQAIR v15.0 to update the LOS.dat format called, convertLOS. Running this command in a folder with an old formatted LOS.dat file will create a new file called LOS15.dat. The LOS15.dat file will need to be renamed to LOS.dat to be used by NEQAIR.

10.2 Convert neqair.inp to v15 format

There is also a utility to update the neqair.inp format called, convert14to15 Running this command in a folder with an old formatted neqair.inp file will create a new file called neqair15.inp. The neqair15.dat file will need to be renamed to neqair.inp to be used by NEQAIR.

11 Usage Recommendations/Notes

11.1 For CFD used as input to NEQAIR

As mentioned, 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, this may cause several orders of magnitude increase in radiation). 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 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 either side to avoid the possibility of the glitch appearing in the spectral region of interest.

11.3 Selecting Grid Types

The default grid type to use is automatic (formerly 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 manual (formerly grid type 0). This means that the user defines the spectral spacing. Running in manual mode can significantly reduce run times compared to running with automatic grid. However, if you plan to run many cases with a manual grid, it is recommended to spot check a couple of calculations by comparing the results obtained with manual and automatic grids to confirm that the manual 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 Expanding/Afterbody Flows

With minimal experimental data for radiation relevant to atmospheric entry encountered in afterbody flows, NEQAIR results have not been as well validated for such regimes. Recent flight data obtained for total heat flux at Mars during the Schiaparelli entry showed good agreement with NEQAIR (Brandis, 2019), suggesting predictions were reasonable at least for this case.

11.5 Passing CFD results to NEQAIR

CFD solutions tend to start with freestream conditions at low temperatures. When passing the results to NEQAIR, it is recommended to only include the CFD results from when T_v 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. Although NEQAIR has been made more robust to low temperature solutions, it is still possible that low temperatures in the freestream may cause errors or failures in the code. If it is found that unreasonable or no solutions are being obtained for your case, check that low temperature points are not included in the LOS.

12 Performance Results

The following two tables list the performance of several recent versions of NEQAIR using the Ivy Bridge nodes on the Pleiades cluster at NASA Ames, both in terms of the body directed radiative heat flux (Table 2) and in terms of the run time (Table 3). NEQAIR v13.1r2 is a version of NEQAIR that contains a few small bug fixes (of v 13.1) in order to confirm results obtained with 13.2. However, 13.1r2 does not contain the additional physics included in v13.2. NEQAIR v15.0 is run two different ways. One way is listed as "(v14.0 inputs)", which runs v15.0 with the same input parameters as was used in v14.0, and thus is the most appropriate row to compare the heat flux results across versions. Results for v15.0 are also listed as "all bands, Auto" and "all bands, Fast". These results use the same input file for all test cases, and include all bands corresponding to the DPLR CFD inputs (using the 'A' option in NEQAIR), and a sufficiently large wavelength coverage (from 855.5 to 200000 A), which was not the case with the v14.0 parameters. These changes to the input file cause an increase in radiative heat flux from "v14.0 inputs" to "all bands". "Auto" corresponds to using an automatic spectral grid, and "Fast" to using the fast (reduced) spectral grid. The "all bands" option has not been run for the MWIR MARS EAST test case, as this test case specifically focuses in on radiation from CO and CO_2 in the MWIR.

Table 2. Radiance for NEQAIR test cases.

Radiative Heating, W/cm^2	Afterbody	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	308.5
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	5.45	20.9	4.8	669.3	33.1	9.3	4000.8	262.1
v15.0 (v14.0 inputs)		20.9	4.8	680.1	30.2	3.5	3689.5	262.8
v15.0 (all bands, Auto)	14.44	22.8	6.0	703.4	30.3	5.3	3663.7	264.3
v15.0 (all bands, Fast)	14.50	22.7	6.0	707.0	30.3	5.3	3769.2	264.3
Percent Difference:								
v14.0 -> v15.0 (v14.0 inputs)		-0.1%	0.0%	1.6%	-9.7%	-168.5%	-8.4%	0.3%
v14.0 -> v15.0 (all bands)	62.2%	8.0%	N/A	4.8%	-9.3%	-75.5%	-9.2%	0.8%
v15.0 (Auto) -> v15.0 (Fast)	0.4%	-0.1%	0.0%	0.5%	0.0%	0.0%	2.8%	0.0%

Table 3. Run times for NEQAIR test cases.

Number of points in LOS	116	78	1	71	58	70	57	118
Computational Time, minutes	**Afterbody Earth**	**CEV**	**MWIR Mars EAST Shot**	**FIREII**	**Mars**	**Titan**	**Venus**	**Saturn**
v14.0	3.08	2.02	0.63	1.62	2.95	1.58	2.10	0.97
v15.0 (as v14.0)		1.85	0.38	0.98	2.00	0.87	1.45	0.57
v15.0 (all bands)	1.97 (Manual grid)	2.73	N/A	1.35	2.78	1.70	2.18	1.22
v15.0 (all bands, Fast, with IS)	0.77	1.07	N/A	0.67	1.35	0.87	1.58	0.97
v15.0 (all bands, Fast, no IS)	0.73	0.92	N/A	0.48	1.05	0.58	1.30	0.37

Note: "IS" refers to whether intensity_scanned.out & intensity.out are written. When running in Fast mode, it would generally be advisable to turn these outputs off.

12.1 Notes on Test Cases

Each test case directory contains the appropriate LOS.dat, neqair.inp and run_neqair.pbs files. To run a test case, copy the directory to your local directory, and submit run_neqair.pbs. There are submit scripts for both SLURM and Torque Maui, set up specifically to be run on the cedar and Pleiades clusters at NASA Ames. 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 between recent NEQAIR releases for each test case.

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 one 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, which is partly validated against EAST data. Some of this increased radiation was later found to be in error as will be noted below.

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

Run times from 13.2 to 14.0 were discussed in v14 release notes but not repeated here. The parallelization of the code permitted significant speed-ups over serial mode.

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

MWIR Mars EAST Shot: No change, as expected.

Mars: The decrease in the intensity is due to the implementation of a non-Boltzmann (QSS) model in v14. Increase due to changes in tangent slab integration and extending the wavelength region out to 60,000 Å offsets this reduction to a small extent.

Titan: The significant decrease in the intensity is due to the implementation of a non-Boltzmann (QSS) model in v14.

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.

12.1.3 From v14.0 to v15.0

Afterbody Earth: New test case for v15.0. The excitation of atomic nitrogen has been updated, and corresponds to a significant increase in the prediction radiation and is now more consistent with HARA. However, solutions for conditions such as this are not yet validated.

Mars: Updates to the QSS model in v15.0 decreased the heat flux by ~9%.

Titan: Adding the N_2 C state to the non-Boltzmann model removed a significant overprediction of radiation from N_2 2nd positive in v14.0.

Venus: Fixing an error in the carbon bound-free calculation (level matching routine) reduced the heat flux by ~9%. By comparison to EAST data, the v14.0 calculation provided an over-prediction of carbon bound-free radiation while v15.0 appears to provide an under-prediction.

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

FIREII, Saturn: Small differences for FIREII due to changes in non-Boltzmann and new levels being added and Saturn due to updates to line broadening.

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14 Description of some NEQAIR Warning and Error Messages

NEQError: emissivity.in range is smaller than requested output range

If emissivity.in is specified as an input, the file must cover the entire wavelength range as specified in neqair.inp.

neqError: Unable to auto-calculate line spacing in region *xxx*

This error can occur if there is no transition corresponding to the *xxx* wavelength range where the minimum line width can be calculated to inform the automatic grid spacing calculation. Try increasing the wavelength range.

Warning: NonBoltz produced a non-physical result. NonBoltz has not been run for *xxx* at LOS *yyy*

If an error is found in the NonBoltz solve, or a non-physical result is found, the solver will switch to run in Boltzmann for that particular line of sight point. This switch will generally occur at low temperature, and as such, should not impact the final radiative heat flux. The change in radiance at the LOS number referenced can be checked to assess the impact.

WARNING: Ion is required. Bound-Free turned off for *xxx*

If a neutral atom, *xxx*, is included in LOS.dat, but not the ion and electrons, the bound-free (and free-free) transitions will be automatically turned off. This message lets the user know, but the calculation will continue. If bound-free radiation was expected for the species referenced, its ion (and electrons) should be included in LOS.dat

WARNING: NonBoltz data not available for *xxx*

If Non-Boltzmann data is not available for a particular atom or molecule, xxx, the transition will be run in Boltzmann, even if the calculation has been selected to run in Non-Boltzmann. This message just lets the user know, but the calculation will continue.

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 points in LOS.dat start at very low vibrational temperatures (i.e. < 500 K), and grid_type is 'A',

the grid can become very large and slow down the calculation; therefore, it is recommended to delete the points up until the vibrational temperature passes 500 K. If grid_type is 'M' and a small delta_lambda has been used, you can try setting grid_type to 'A', or increasing delta_lambda. However, care must be taken in order to ensure that delta_lambda is not set so large that there will not be enough points to correctly describe each spectral line. This may be checked by trying multiple values of delta_lambda (i.e. grid convergence).

WARNING: Stark broadening parameters not available for *xxx*

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

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. If XXX is not a species specified in LOS.dat, the file headers were not formatted correctly and this indicates a read error.

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. If XXX is not a species specified in LOS.dat, the file headers were not formatted correctly and this indicates a read error.

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 the solution to the Saha-Boltzmann equation in 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. While this might be an input error for compressive flows, in backshell/expanding cases it is typical to obtain very large electron overpopulations and this warning may occur frequently in those cases.

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: 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.

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 was done intentionally, the user may recompile the code with a sufficiently large MaxPoints constant. If not, 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
ERROR: Lines to TOP level matching failed
ERROR: Top Base level degen does not match LEVELS.dat degen
ERROR: QSS Term list does not match degeneracy
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, LINES_ATOMS.dat and LEVELS_ATOMS.dat. Restore the DATABASE files and if this error persists, contact the NEQAIR developers.

The # electronic diatomic band systems entered > MaxBands
The # IR diatomic band systems entered > MaxIRbands
Number of molecules in qssm calculation > MaxDiatom
 # dissociation cross-sections > MaxMolStates
'# electronic transitions > MaxMolTrans
No. of atomic systems entered exceeds MaxAtoms

These error messages indicate that there are more bands/states/transitions requested in either a v14 neqair.inp or in the databases than it is currently setup to handle. If databases were modified, these constants may be updated and the code recompiled. If

not, verify that extra items have not been added to neqair.inp and/or switch to v15 format. 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.

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*
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 solveNonBoltz; *xxx*

This error indicates that a unique solution to the QSS equations cannot be found. In the v15.0, the solver should switch to Boltzmann in such situations, so this area may no longer occur in practice. This may sometimes be caused by low temperature points in LOS.dat. Verify the input files (LOS.dat) are correct.

Unable to open LEVELS_ATOMS.dat database file. Expected path name: *xxx*
Unable to open LINES_ATOMS.dat database file. Expected path name: *xxx*
Unable to open EXCITE_ATOMS.dat database file. Expected path name: *xxx*
Unable to open LEVELS_MOLE.dat database file. Expected path name: *xxx*
Unable to open LINES_MOLE.dat database file. Expected path name: *xxx*
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 is correct, please check that EXCITE_ATOMS.dat, LINES_ATOMS.dat, LEVELS_ATOMS.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.

Unable to open file CDSD_CO2.txt

This error indicates that the CO_2 IR band system was turned on, but NEQAIR 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