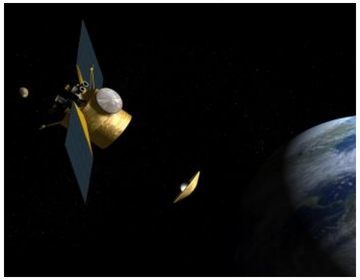
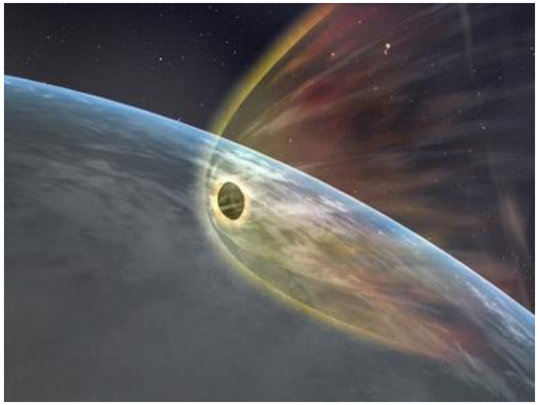
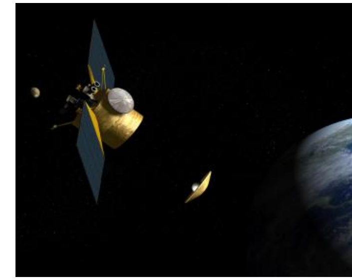


NEQAIR v14.0 User Tutorial

Aaron Brandis and Brett Cruden

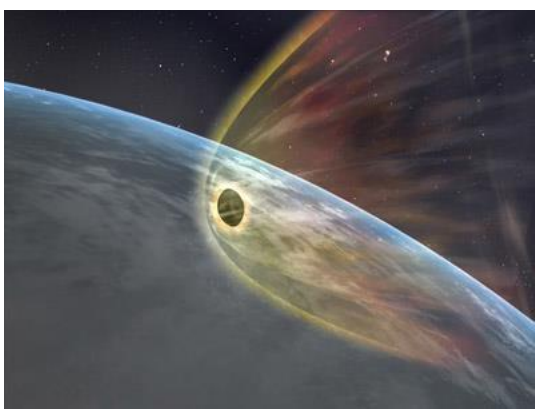




NEQAIR v14.0 User Tutorial

Aaron Brandis and Brett Cruden

Code contributions: Chul Park, Jim Arnold, Ellis Whiting, John Paterson, Lily Yang, Grant Palmer, Dinesh Prabhu, David Saunders, Yen Liu & others

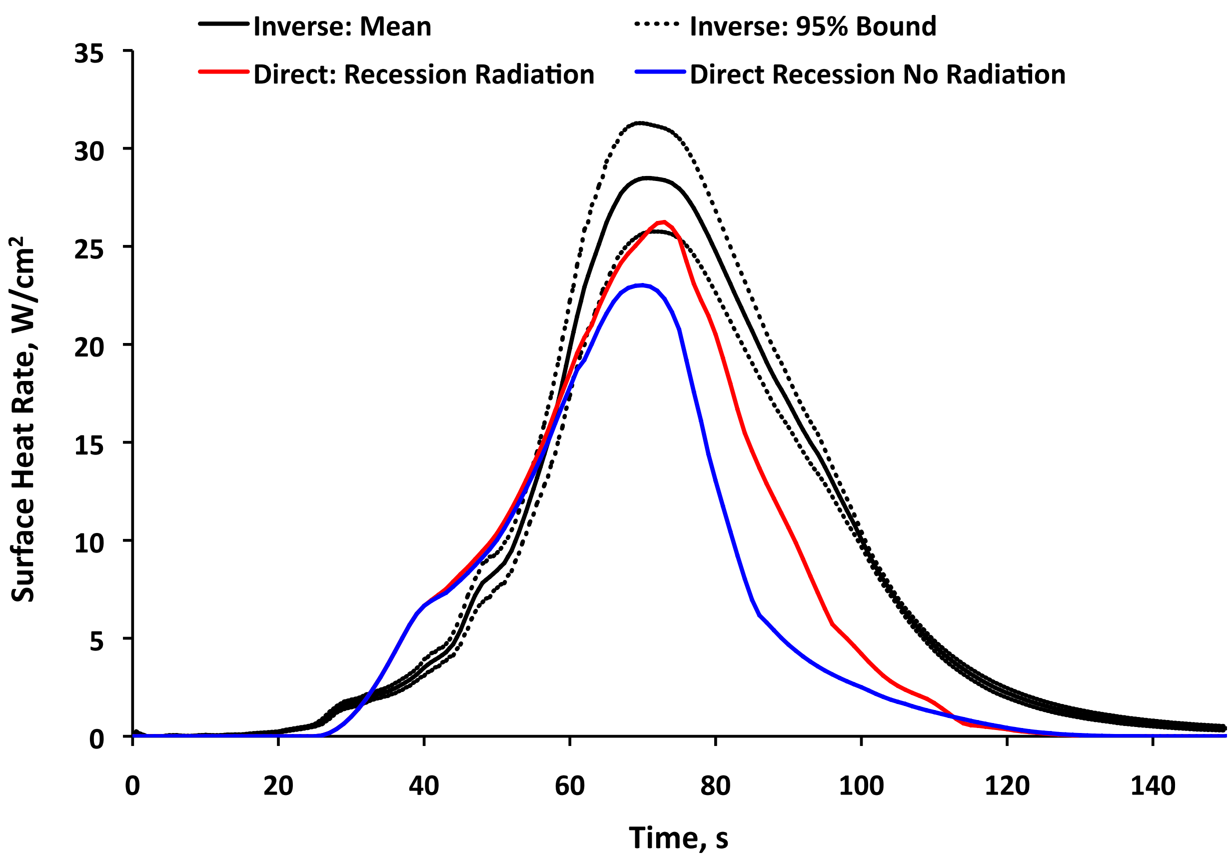


Radiative Heating For Flight Missions

- Radiative heating plays two main roles relevant to mission design:
  1) Calculating the radiative heat flux incident on the surface of an entry vehicle.
  2) Validating these results within quantified uncertainty bounds with experimental data to help evaluate margin policies.
- Subsequently, there are two principal modes for running NEQAIR:
  1) As a radiative heat flux prediction tool for flight projects (also has been used to simulate the radiance measured on previous flight missions).
  2) As a tool for creating synthetic spectra of any desired resolution (including convolution with a specified instrument/slit function). This mode is typically used in simulating/interpreting spectroscopic measurements of different sources (e.g. shock tube data, plasma torches, etc.).

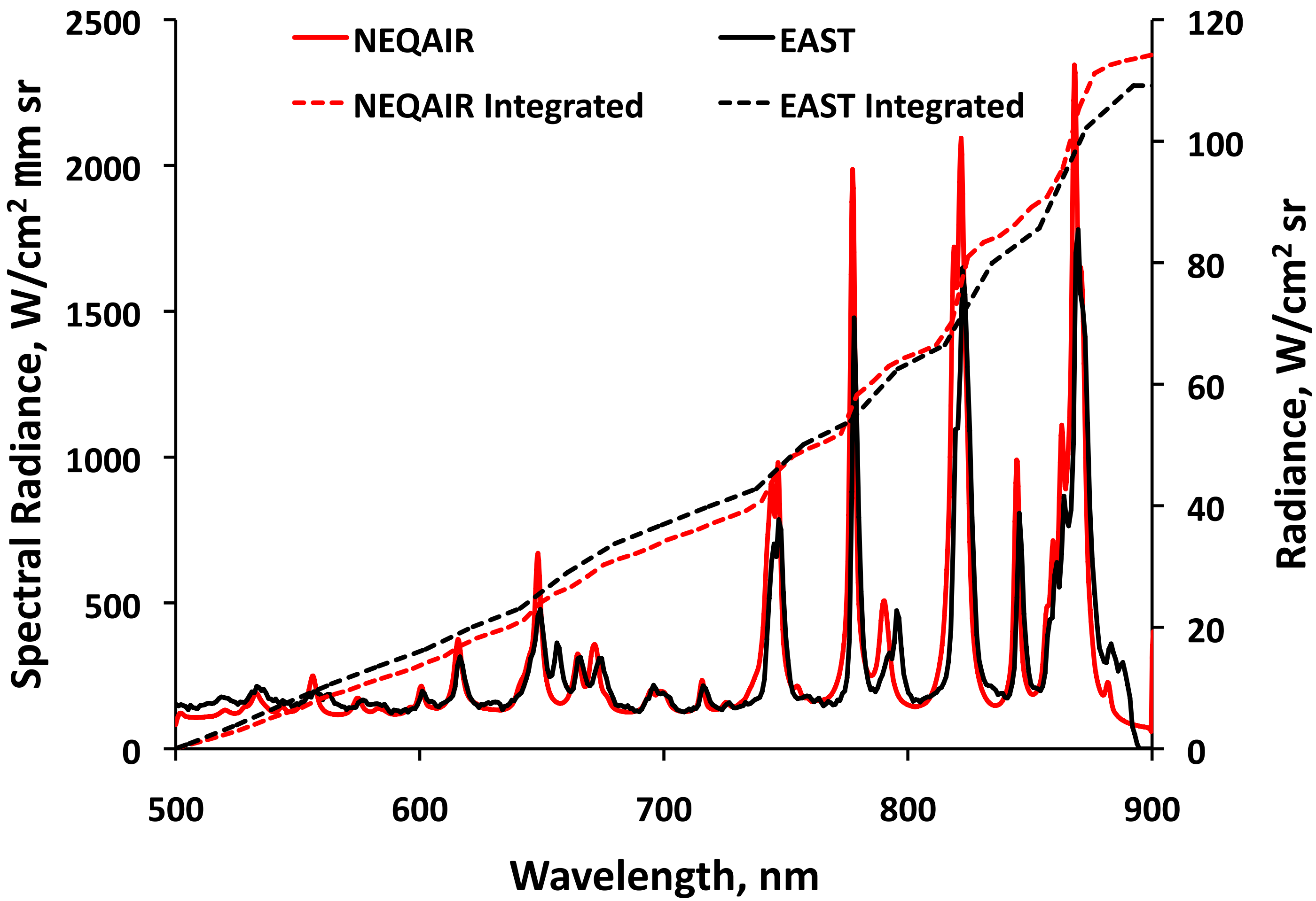
Example of NEQAIR Flight Calculation

- Comparison of NEQAIR & DPLR calculations with the derived heat flux from the Mars Science Laboratory (MSL):



Example of NEQAIR Shock Tube Calculation

- Comparison of NEQAIR with high speed Earth shock tube data from EAST:



NEQAIR

- NEQAIR has been NASA's main radiation code for the last 30 years. It is a line-by-line radiation code that computes spontaneous emission, absorption and stimulated emission due to transitions between various energy states of chemical species along a line-of-sight.
- There have recently been many substantial upgrades to NEQAIR. Both in terms of the physics and the efficiency of running the code.

- **Overview of talk:**
  - Version history of NEQAIR.
  - Describe input/output files and highlight new features.
  - Show improvements in run-time with NEQAIR test cases.
  - Detail the spectral output from test cases.
  - Provide some user recommendations for running the code.
  - Who is allowed to get the code, and how to get it.

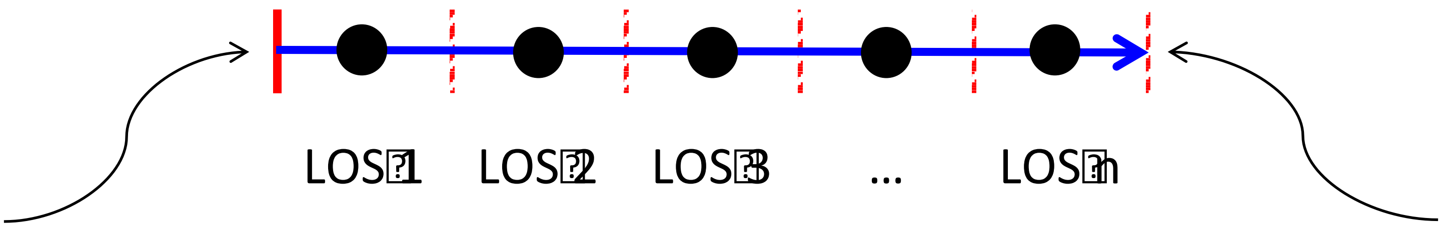
Brief Version History

- **Approximately 22 release versions of the code:**

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

Input Data For Calculation

For each LOS point: x, Tt, Tr, Tv, Te, species number densities are needed at each Line of Sight point (usually provided by a CFD code).

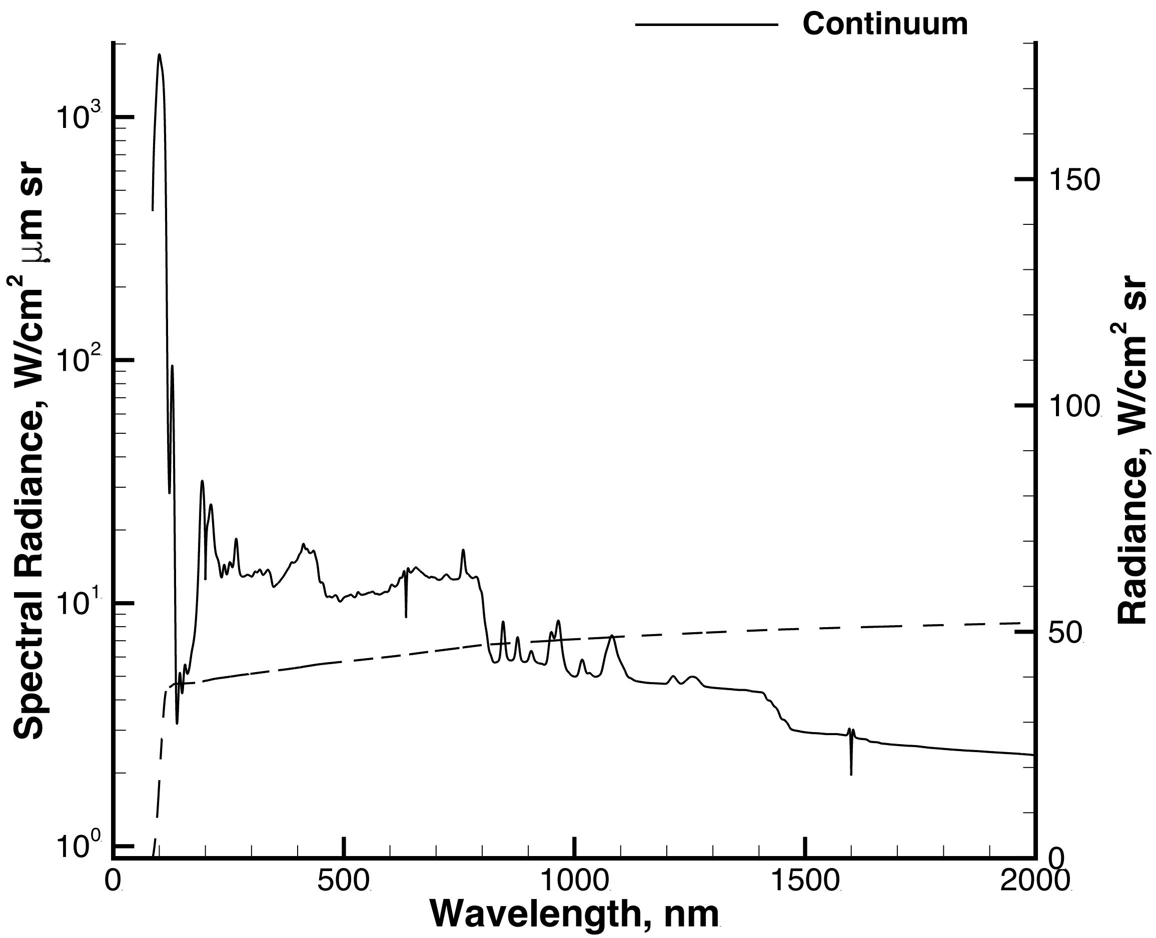


- Intensity.in can used to apply a defined spectral radiance at the first line of sight point.
- A black body can also be specified at the first line of sight point.

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

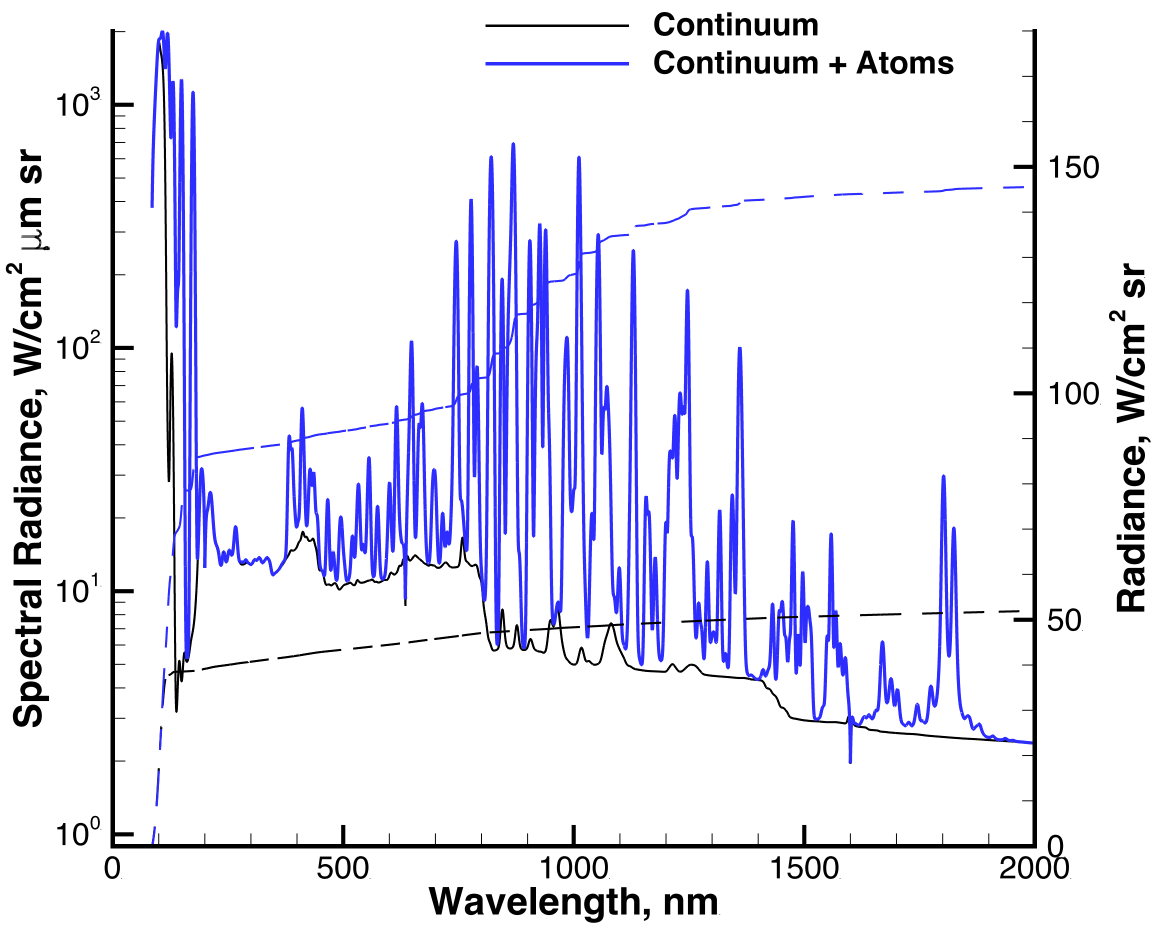
Building a Spectrum

FIRE II Test Case



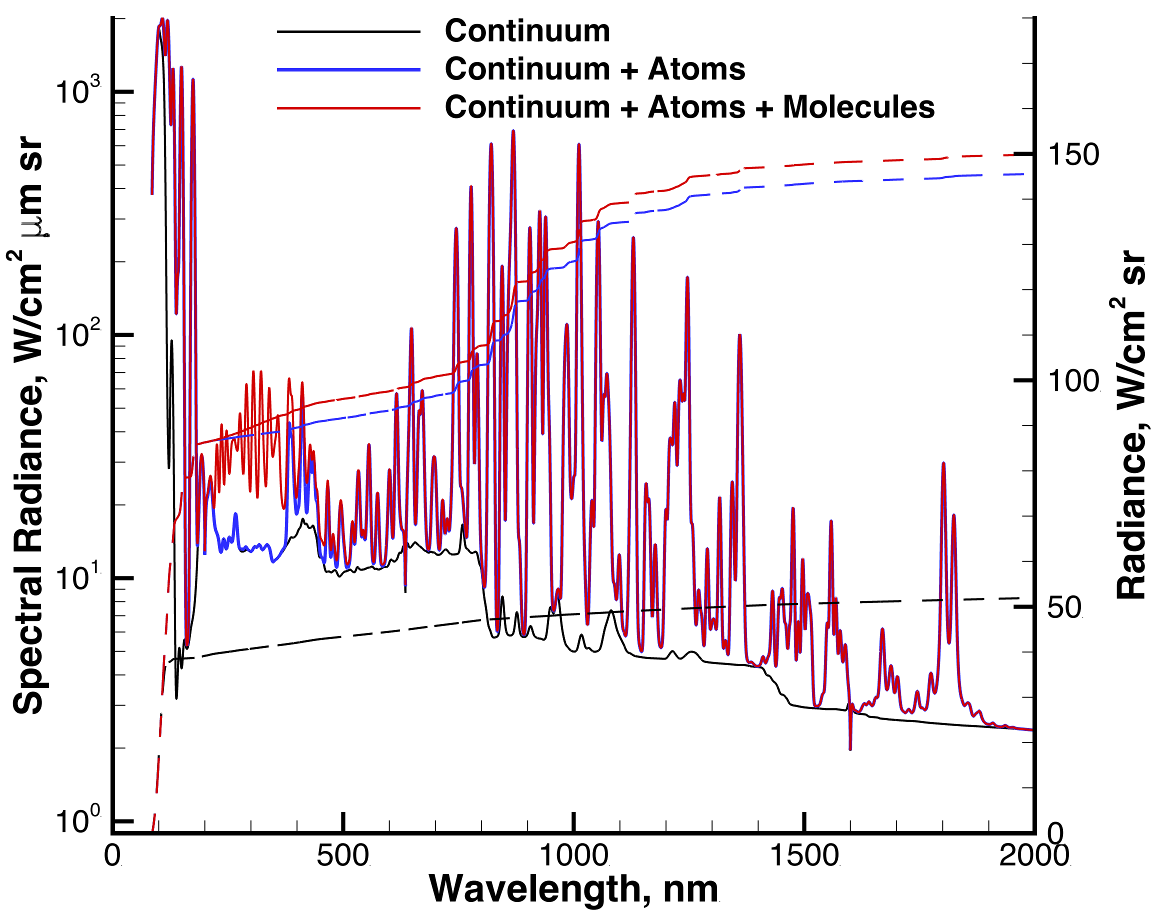
Building a Spectrum

FIRE II Test Case



Building a Spectrum

FIRE II Test Case



Input File: neqair.inp


```
********************************************************************************
                    CEV Test Case
aaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaaa <- 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
********************************************************************************
```

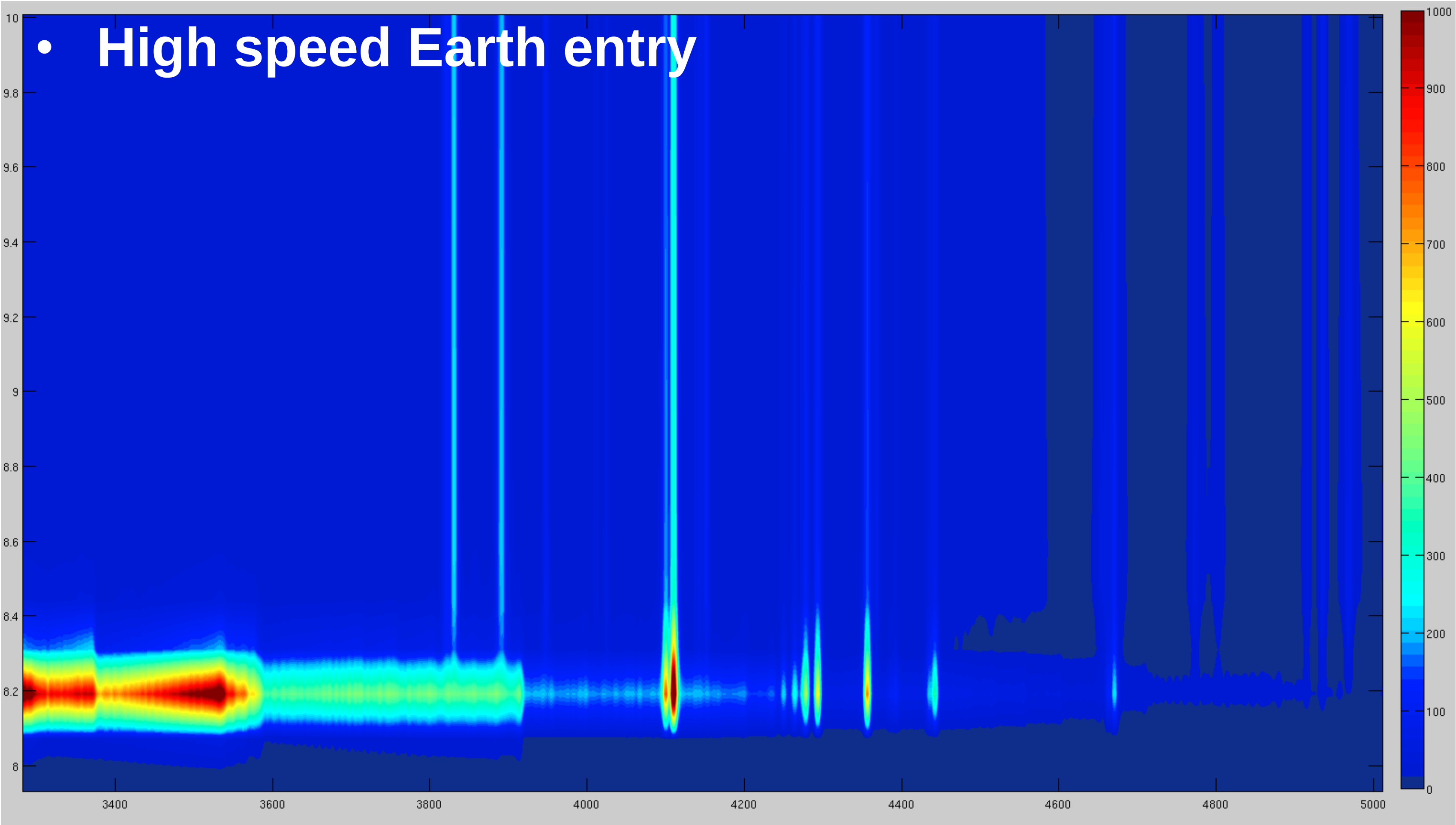
```
PATH TO DATABASE FILES   :  /share/apps/neqair/v14.0/DATABASES/
Line2                                           a
--------------------------------------------------------------------------------
```

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

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

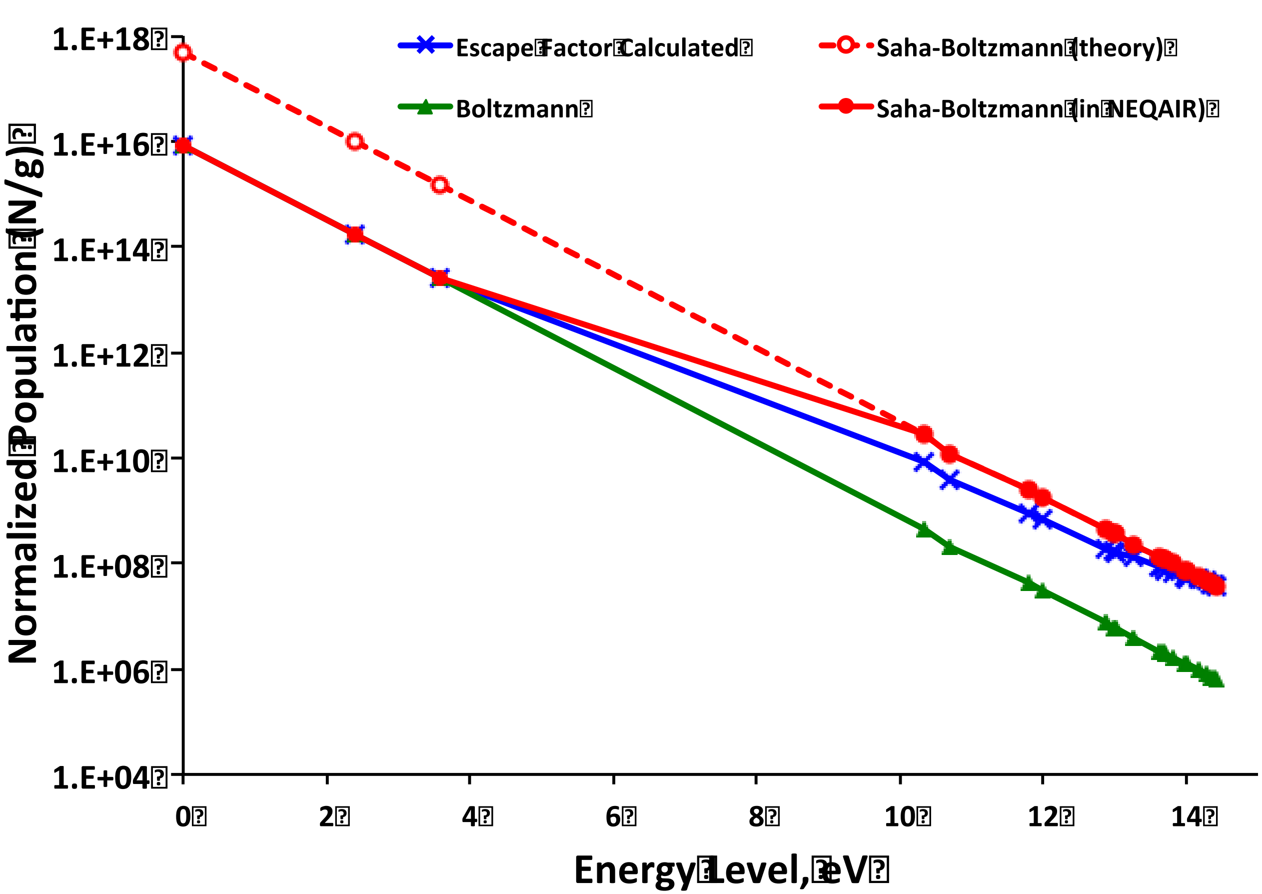
Scan Only: Scans a previously calculated intensity.out file – no radiation calculations are performed

Output Files: 2-D intensity_scanned.out

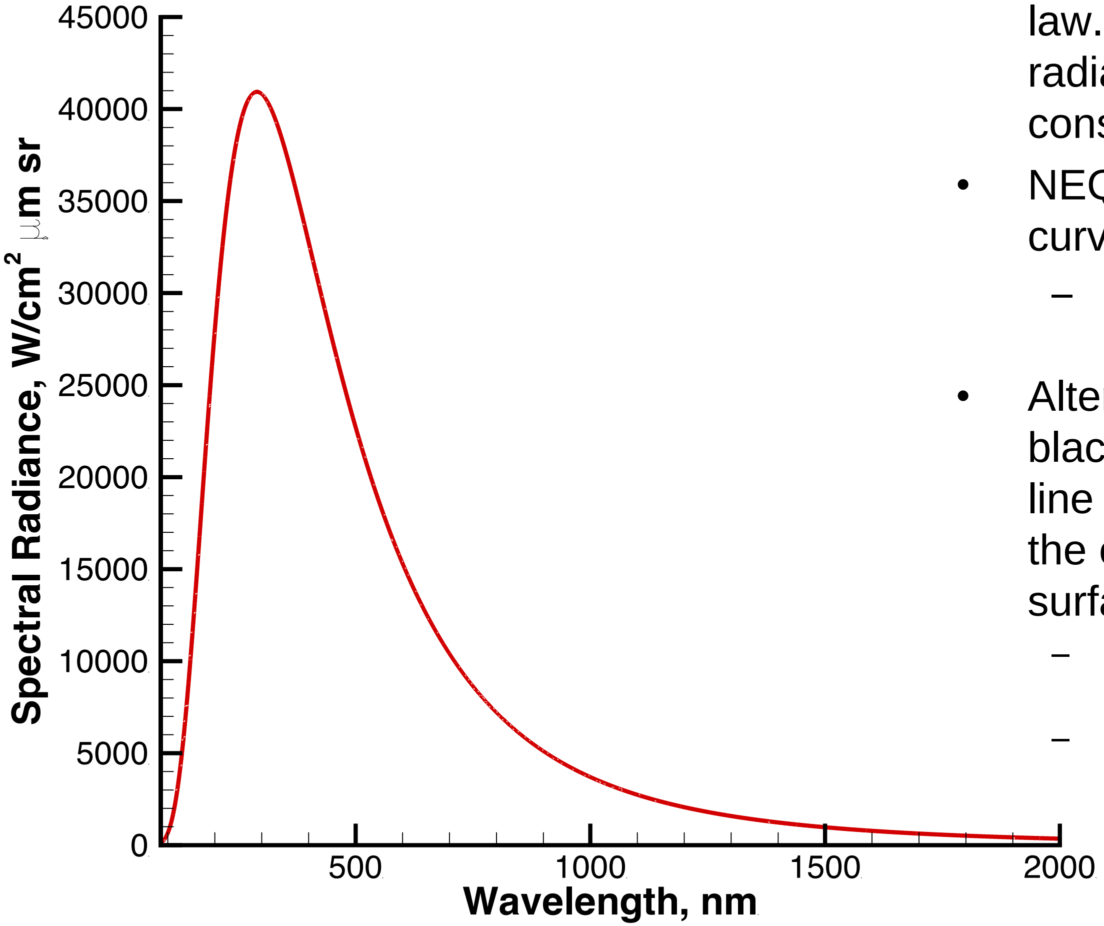


Distributions of Energy Levels

- Different population options for NEQAIR:
  - Saha-Boltzmann
  - Boltzmann
  - QSS using a calculated escape factor
- Example is shown for an expanding flow (ie Saha > Boltzmann)
  - Opposite trend to compressing flows



Black Body



- A black body in thermal equilibrium emits radiation according to Planck's law. It is the theoretically maximum radiation emitted at any given constant temperature.
- NEQAIR can calculate a black body curve for a specified temperature.
  - Achieved by selecting black body, and no other options in line 4.
- Alternatively, NEQAIR can define a black body to be imposed at the first line of sight point (e.g. approximating the emission from a solid heat shield surface)
  - Achieved by selecting black body, along with another option in line 4, such as QSS.
  - For any radiance other than a black body to be defined at the first line of sight point, intensity.in can be used.

Input File: neqair.inp


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

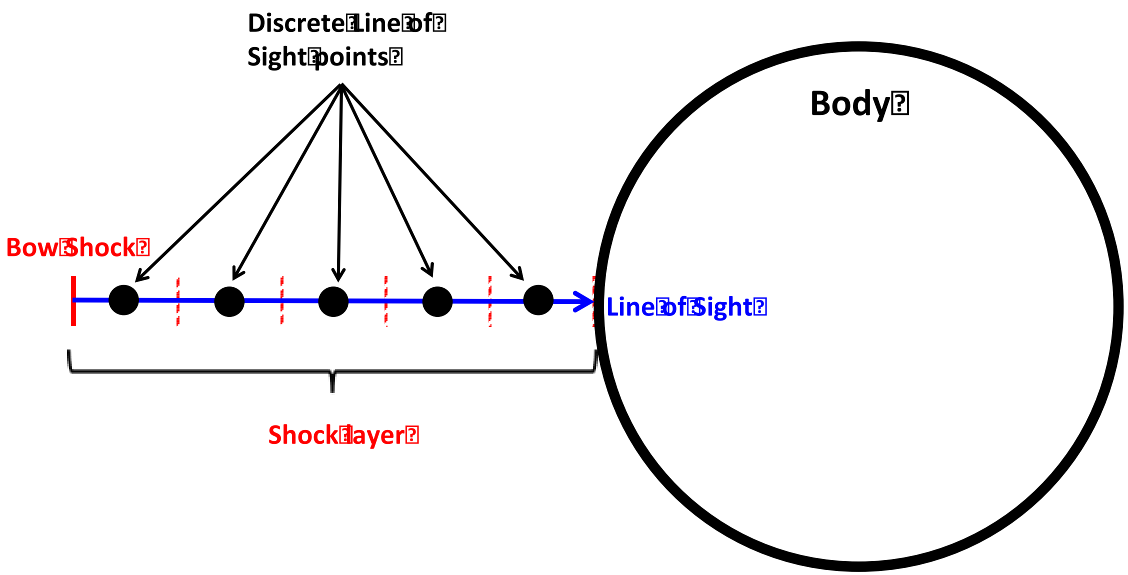
```
FOR STAG PT. :Infinite Slab X; Sphere. Cap 0;  Rnose=  0.0 cm;  Shock Div= 0.0
Line6                        a              a        rrrrrr                rrrrrr
-------------------------------------------------------------------------------
```

```
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
```

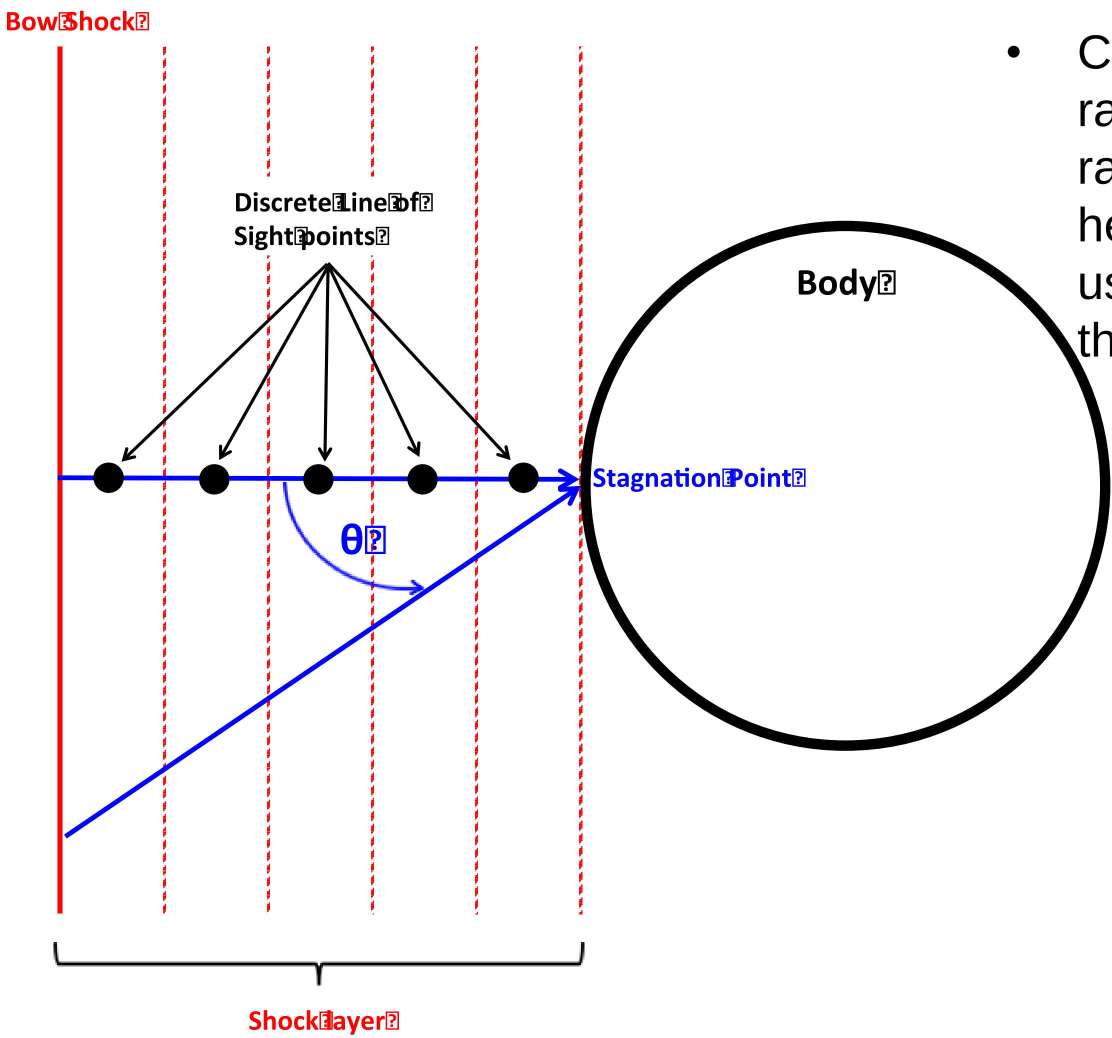
```
   For non-local calc, specify surface : E 1.00, T 0.00 (note: A=E, R=1-E-T)
        (E=emissivity, T=transmittance)     rrrr    rrrr
              :Diatomic Electronic Transition Systems
```

Line of Sight Calculation

- Calculates the radiance and spectral radiance at the stagnation point.

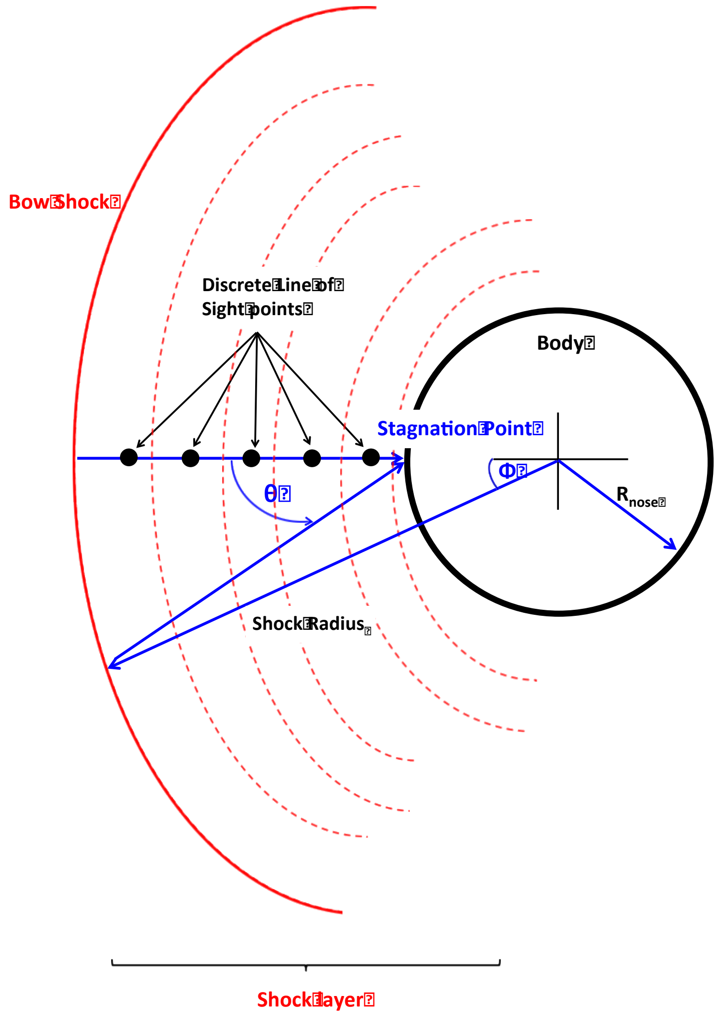


Stagnation Point Calculation



- Calculates the radiance, spectral radiance. Wall-directed heat flux is evaluated using tangent slab at the stagnation point.

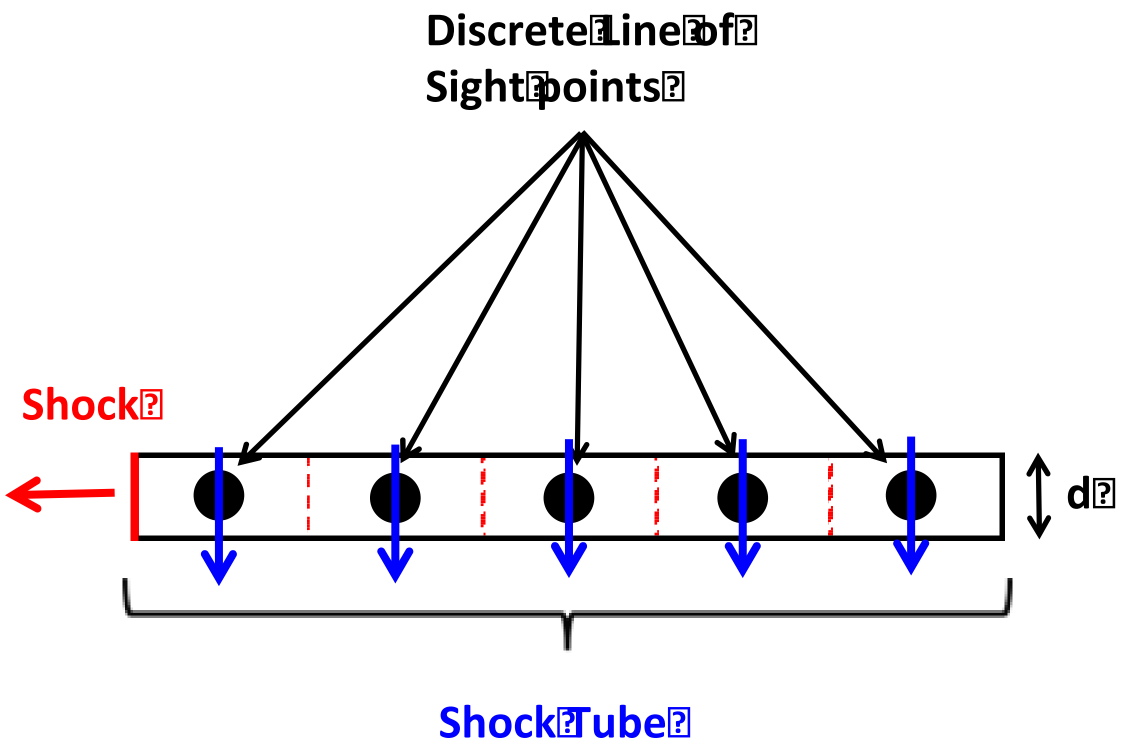
Spherical Cap Calculation



- Calculates the radiance, spectral radiance and wall-directed heat flux at the stagnation point for a spherical geometry.

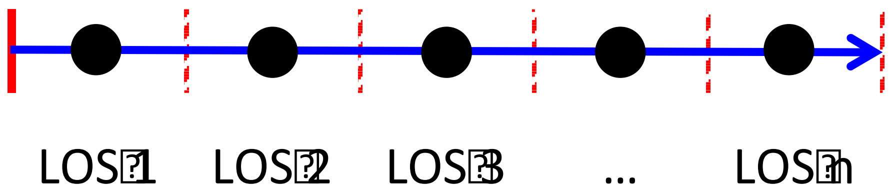
Shock Tube

- Calculates the emission normal to the line of sight direction.



Radiative Transport

For each LOS point: x, Tt, Tr, Tv, Te, species number densities are needed



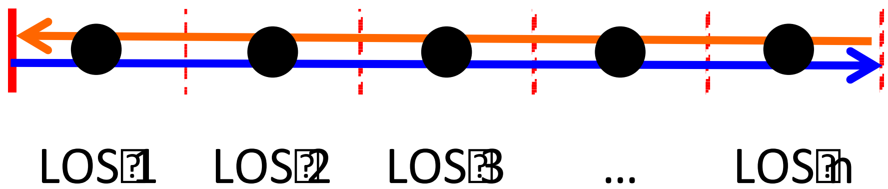
- Exact radiative transport calculations are complicated due to the coupled nature of the emitted and absorbed photons from each of the line of sight points.
- The radiation emitted and absorbed at every point in the flow field is coupled to the radiation emitted and absorbed at every other point.
- An approximate approach used to bypass this complicated coupled problem, is to use **escape factors.**

Escape Factor

- The escape factor is the probability that a photon emitted at a point in a radiating flow field will **NOT** be absorbed after traveling a defined distance through a uniform gas with an effective volumetric absorption coefficient equal to that point of emission.
- NEQAIR has several options for evaluating the escape factor:
  - Have the escape factor calculated by the code *(most common option)*.
  - Have the escape factor set to a specified value between 0 and 1.
  - Perform a non local iterative calculation to avoid using the escape factor assumption for atoms, escape factor presently still needs to be calculated for molecules.
- Escape factor is only applicable for QSS regions (ie not needed for Boltzmann, equilibrium calculations)

Radiative Transport

For each LOS point: x, Tt, Tr, Tv, Te, species number densities are needed

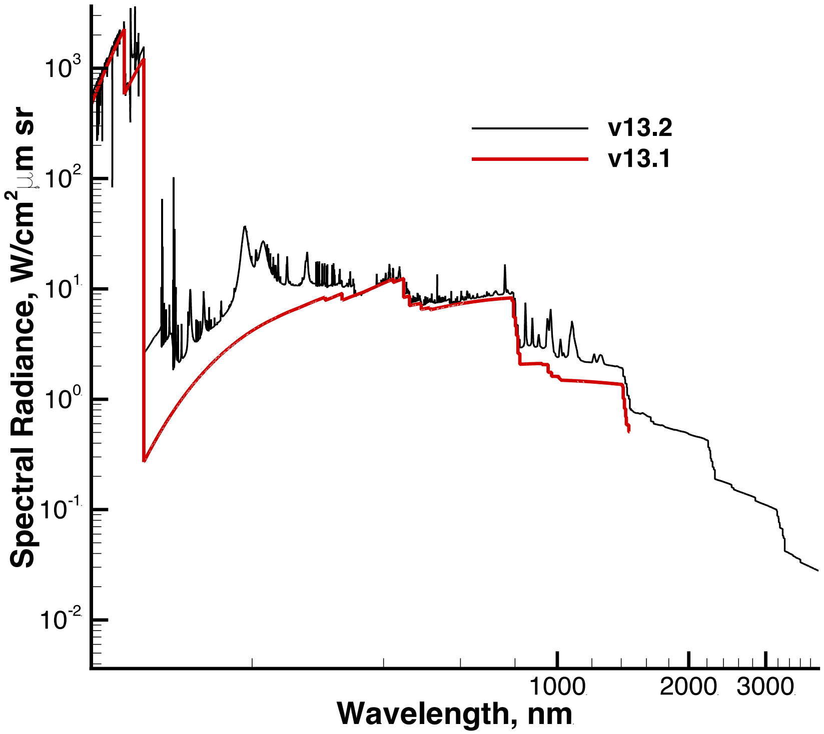


For Non Local calc emissivity data must be specified.

- NEQAIR v14.0 can now iteratively solve the radiation in both directions along a line of sight, and thus not use the escape factor assumption (only for atomic radiation at present).
  - This is now feasible due to the parallelization of the code.

Bound-free TOPBase Update

Entry Systems and Technology Division

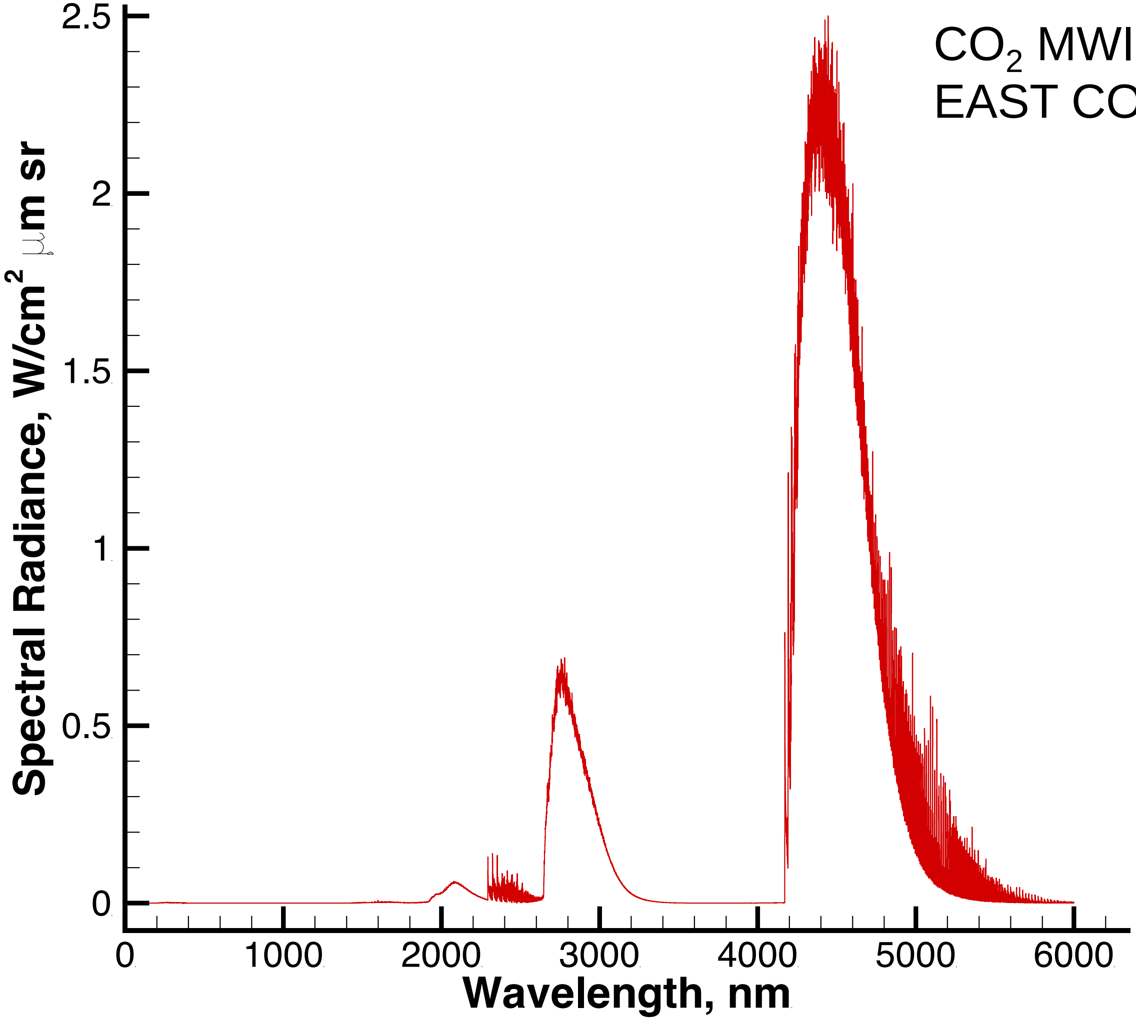


- CEV test case, nitrogen bound-free only.
- Full CEV test case increased from 19.4 W/cm^2 (v8) to 20.8 W/cm^2 (v14.0): 7% change. [6.4 km/s, 45 km]

Input File: neqair.inp


```
                                            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.
```

MWIR CO_2 Radiation



CO_2 MWIR radiation from EAST CO_2 test case

Input File: neqair.inp

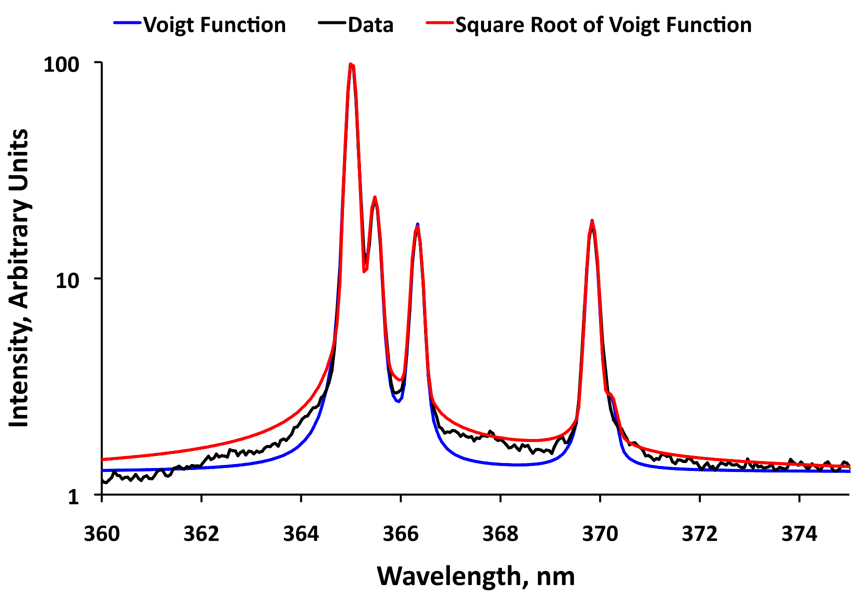

```
REGION DATA:        Line8                       # of regions =   4
                                                               iii
   w1 [A]    w2 [A]    range   grid_type  delta_lambda   pointsPerLine
   855.5    2000.0      600        1        0.00133          10
  2000.0    6350.0       50        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
```

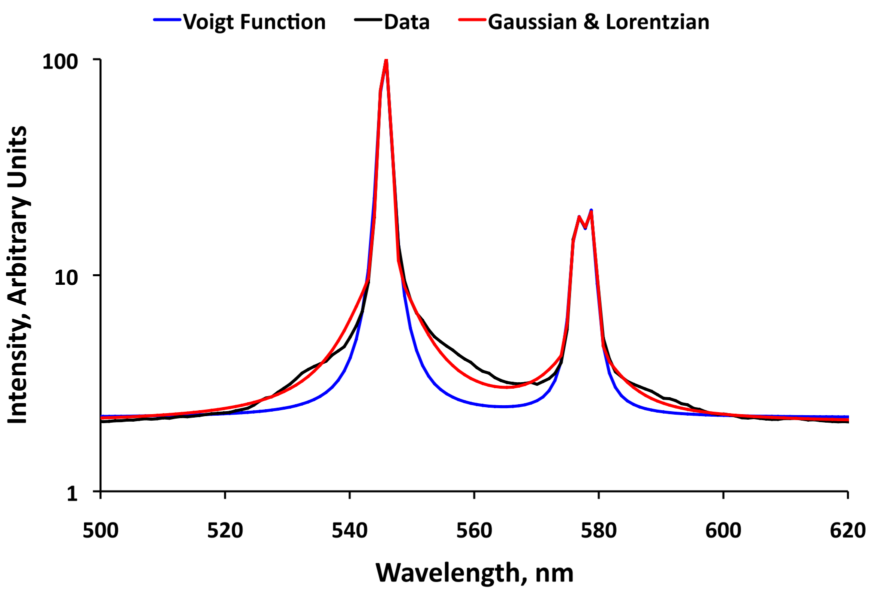
```
SCAN DATA:          Line9        Perform Scan X
                                              a
Slit Function (Voigt,ICCD1,etc) : Voigt    Spectral interval [A] = 0.1
                                  aaaaaa                           rrrrr
Slit Parameters:
      6.0   0.0     2.0       Voigt
   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

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

Different Line Shapes

Entry Systems and Technology Division

- Comparison of a different line shape options compared with a Voigt function and EAST





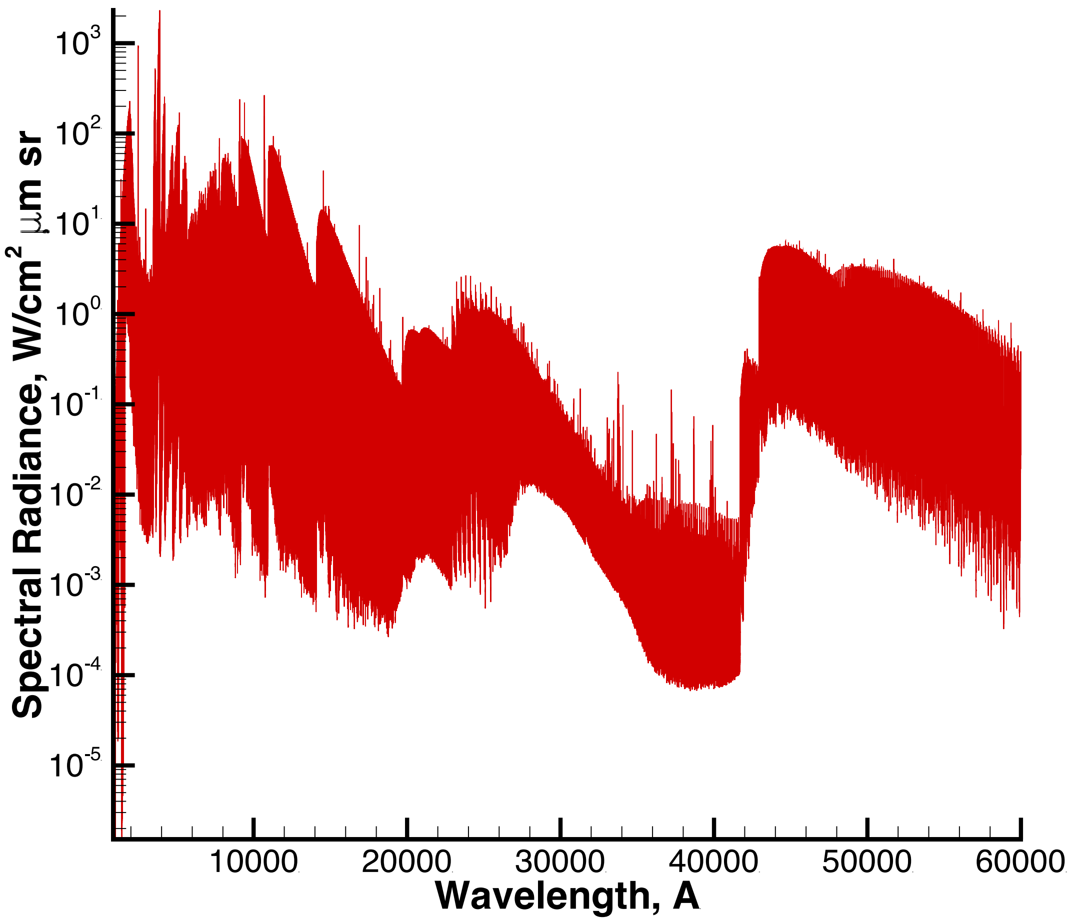
Input File: LOS.dat


```
****************************************************************************
                   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 rrrrrrrrrrrrrr rrrrrrrrr rrrrrrrrr rrrrrrrrr rrrrrrrrre15.6,4f10.1
      rrrrrrrrrrrrrr rrrrrrrrrrrrrr rrrrrrrrrrrrrr rrrrrrrrrrrrr   (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
```

Output Files: intensity.out

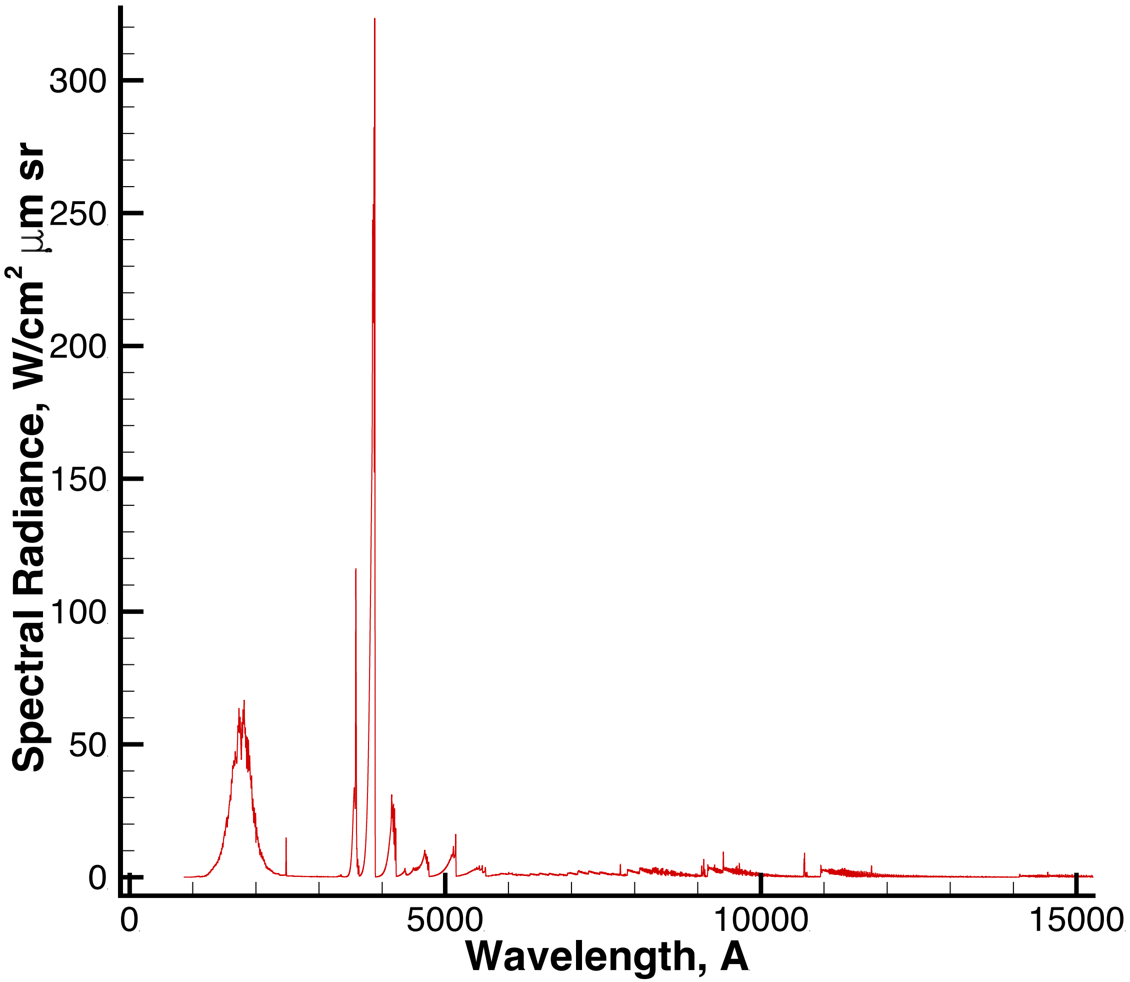
Entry Systems and Technology Division

- Mars test case
- Intensity.out provides high resolution spectra.
- Allows for a detailed comparison between different solutions or between different codes.



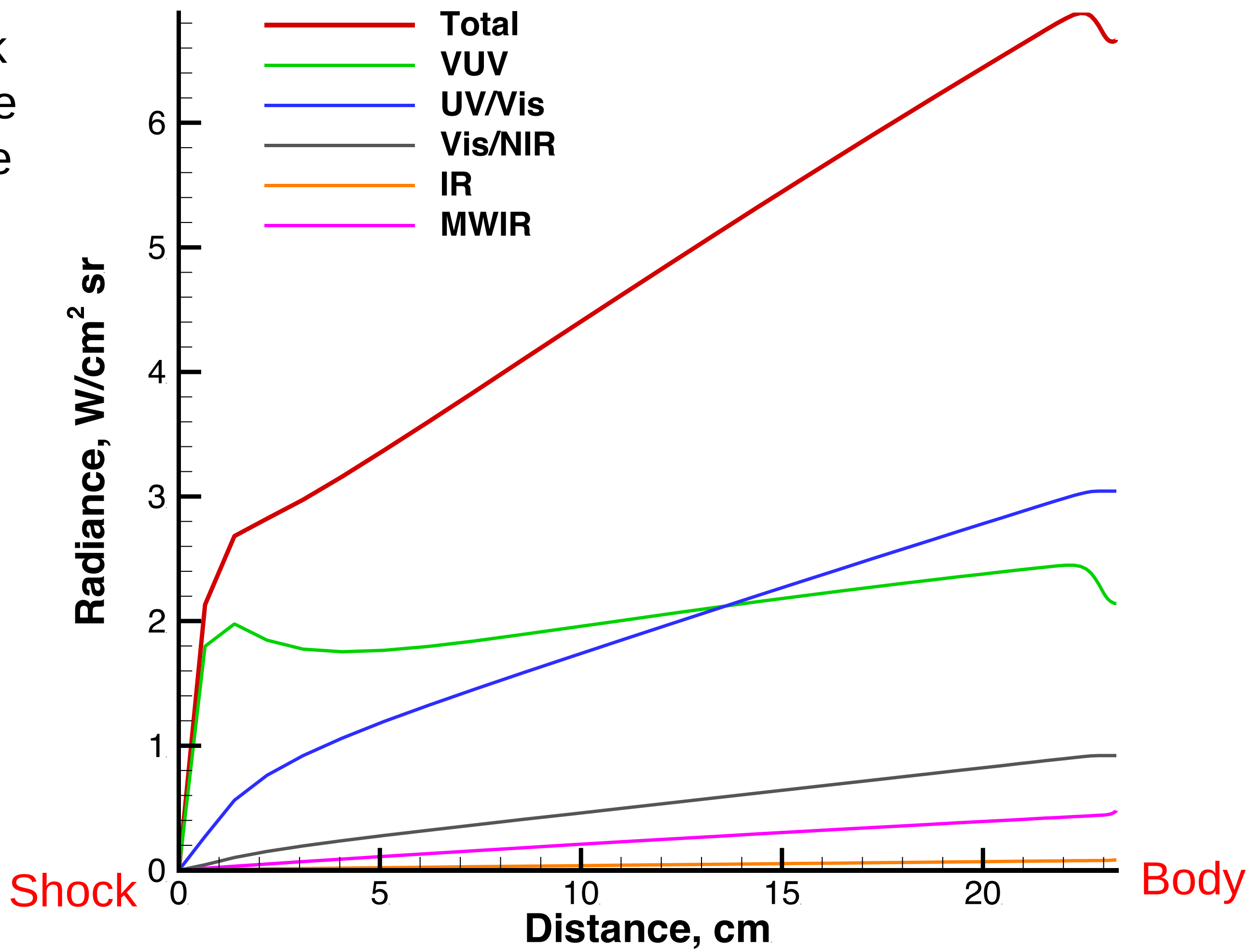
Output Files: intensity_scanned.out

- Mars test case
- Intensity_scanned.out, provides the results of convolving intensity.out with a scan function defined in neqair.inp
- The scan function is usually an approximation of an experimental line shape.
- Allows for more robust comparisons between simulations and experimental data.



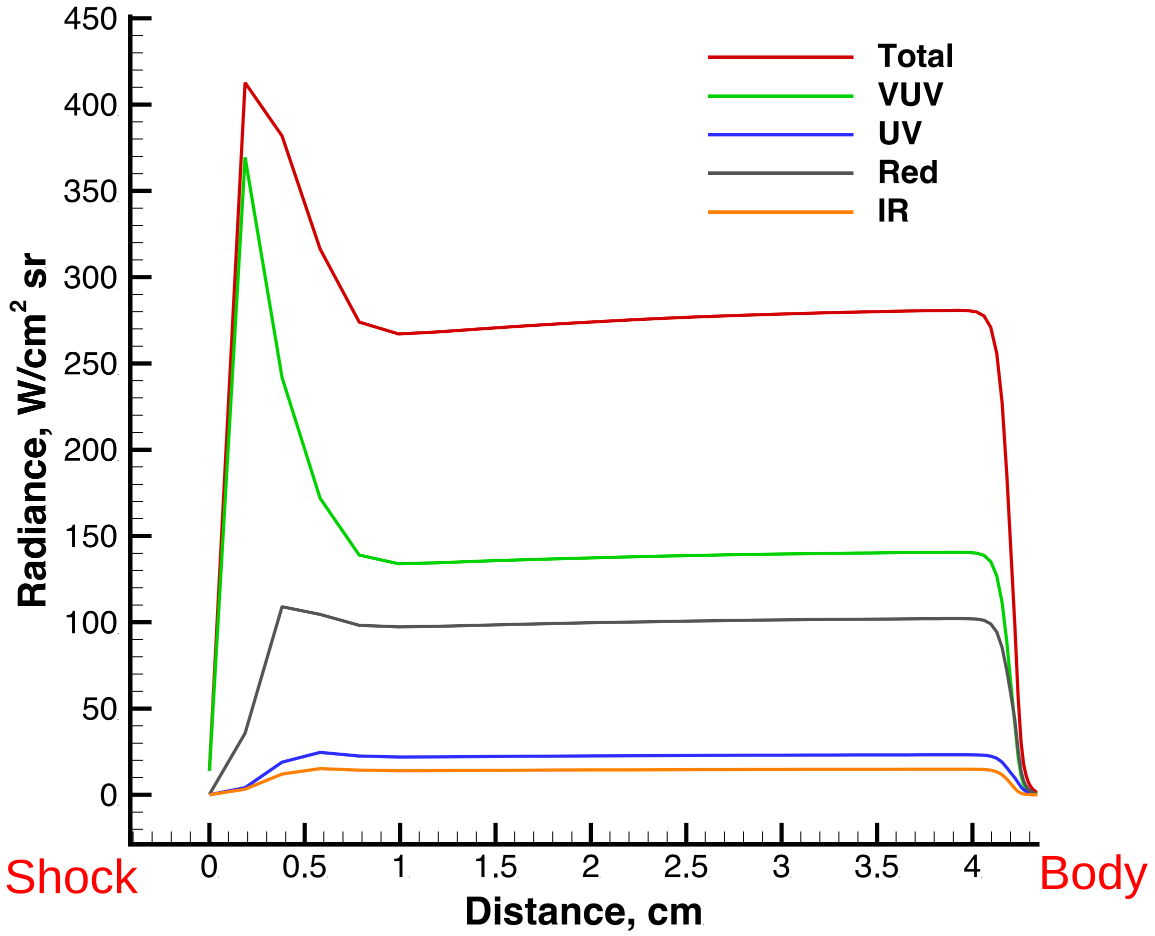
Output Files: LOS.out

- Mars test case
- LOS.out (not in shock tube mode) shows the wall-directed radiance as a function of distance



Output Files: LOS.out (shock tube mode)

- FIRE II test case
- LOS.out (in shock tube mode) shows the radiance normal to the line of sight direction as a function of distance



Output Files: neqair.out


```
                      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
```

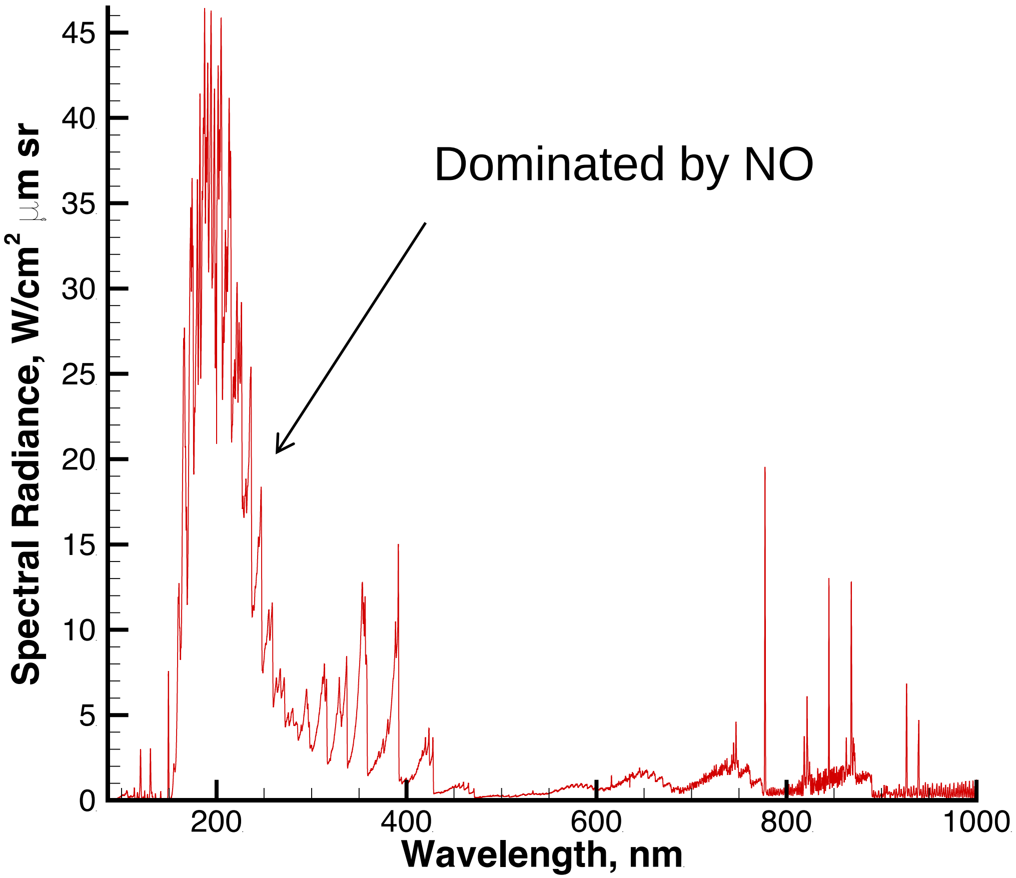
```
Warning: ne of 1.3E+12 is more than 100x greater than the Saha limit at  2166 K
Radiative heating from   855.50 to  2000.00 angstroms =  0.791184E+01 W/cm2
Radiative heating from  2000.00 to  5800.00 angstroms =  0.166056E+02 W/cm2
Radiative heating from  5800.00 to 16000.00 angstroms =  0.560963E+01 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
```

NEQAIR Test Cases: Computational Time

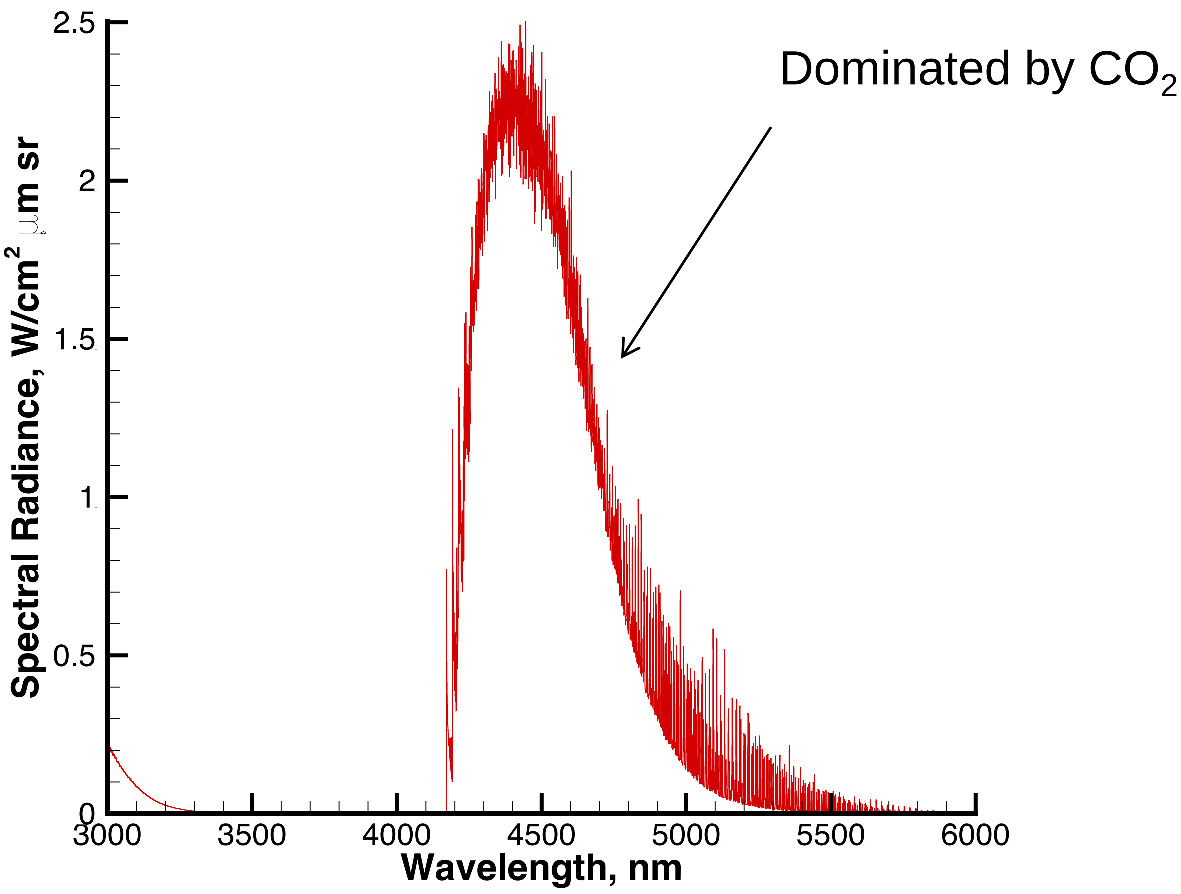
Number of points in LOS	78	1	71	58	70	57	118
Computational Time, minutes	**CEV**	**MWIR Mars EAST Shot**	**FIREII**	**Mars**	**Titan**	**Venus**	**Saturn**
v13.1	40	2.5	18	53	22.5	23.5	32
v13.1r2				53		16	28
v13.2	140	1.5	89	211.5	22	74	20
v14.0 (processors=#LOS)	2.4	1.1	1.9	4.9	0.9	2.5	0.9
v14.0 (1 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**

- NEQAIR can be run for a variety of atmospheric compositions as evidenced by this table (e.g. N_2/O_2, CO_2/N_2, N_2/CH_4, H/He).
- This means that NEQAIR can calculate radiative heating for any given flight mission of interest.
- All test cases now run in just a few minutes.

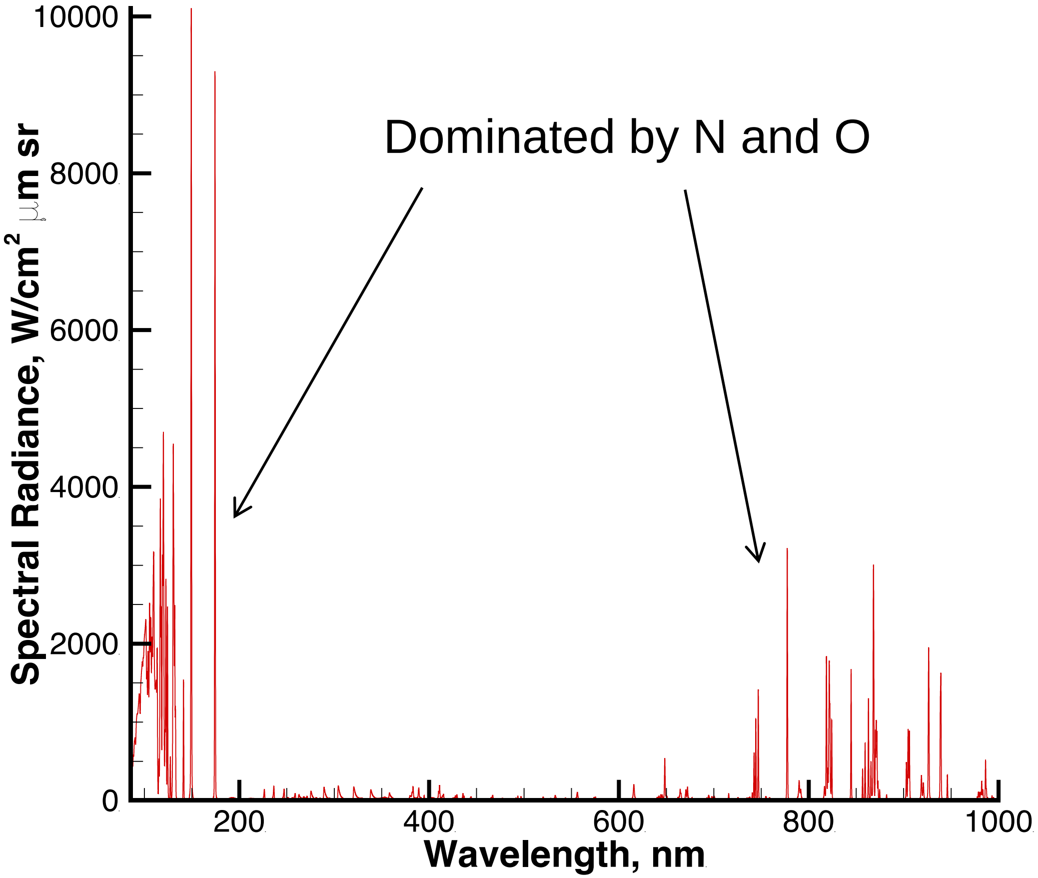
CEV Test Case



MWIR CO_2 EAST Test Case

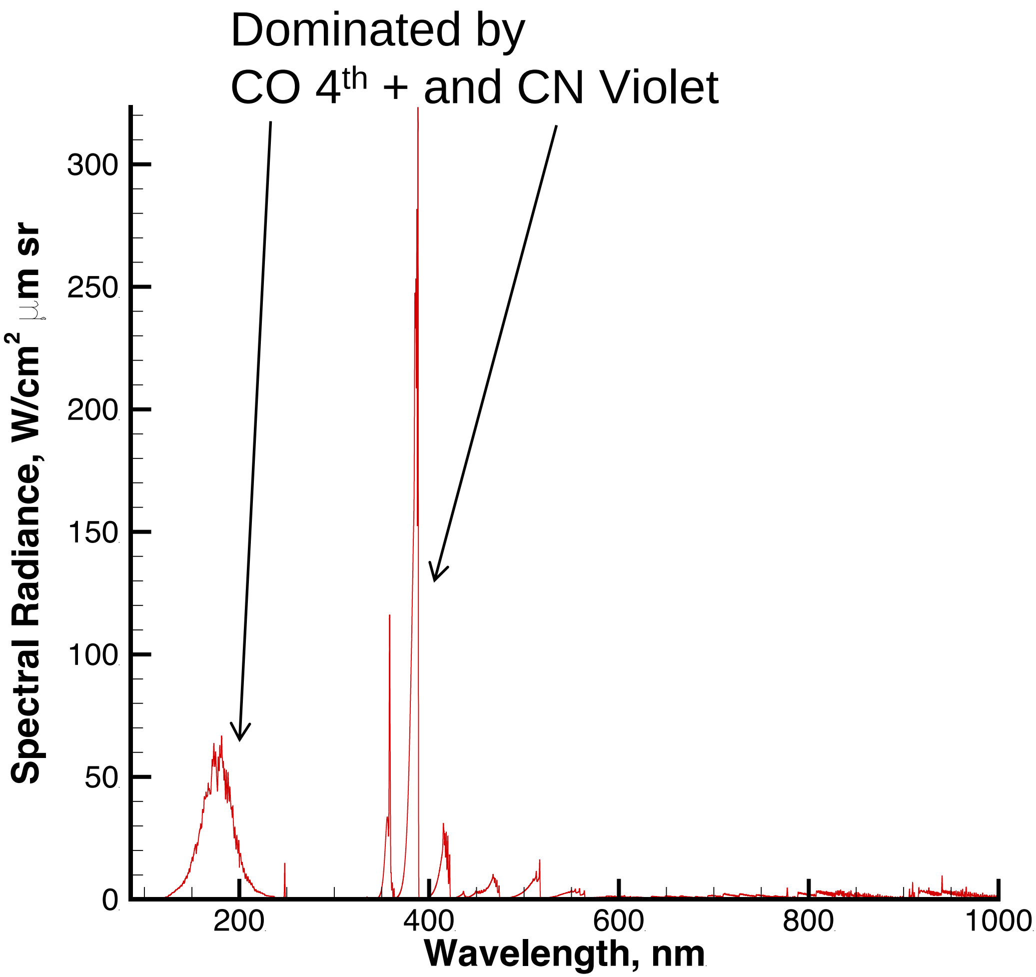


FIREII Test Case

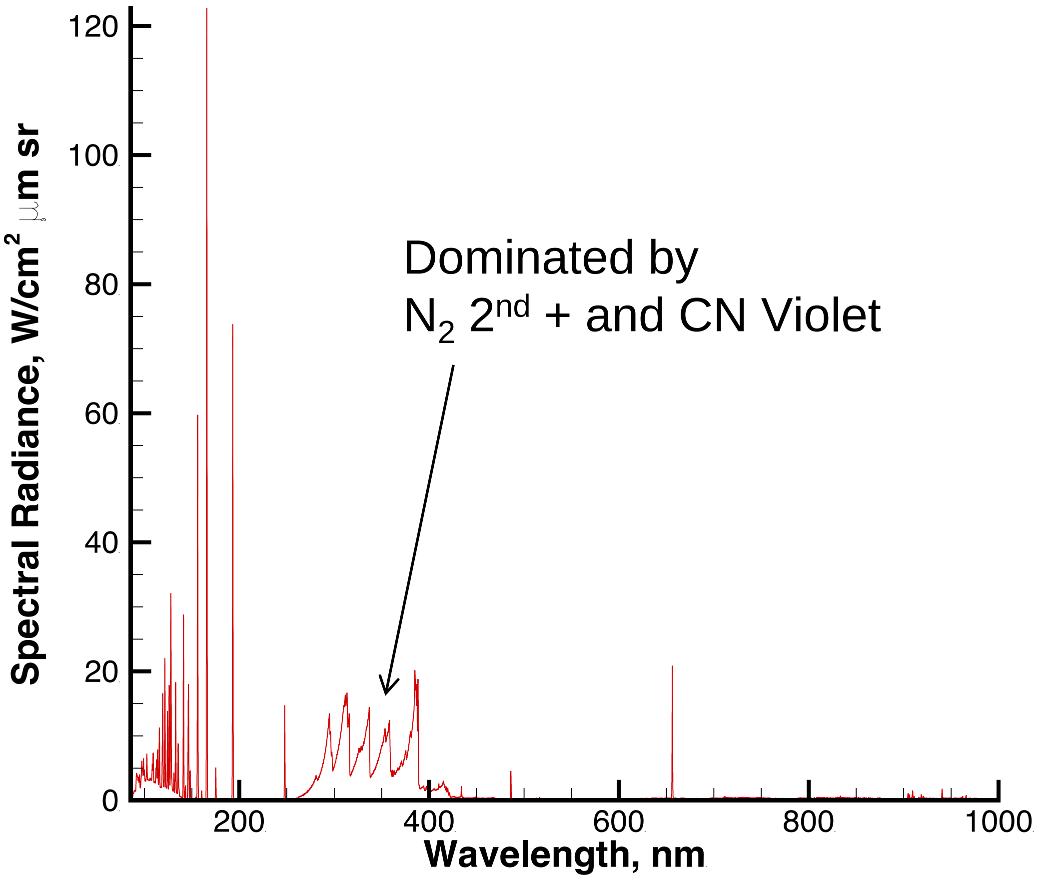


Mars Test Case

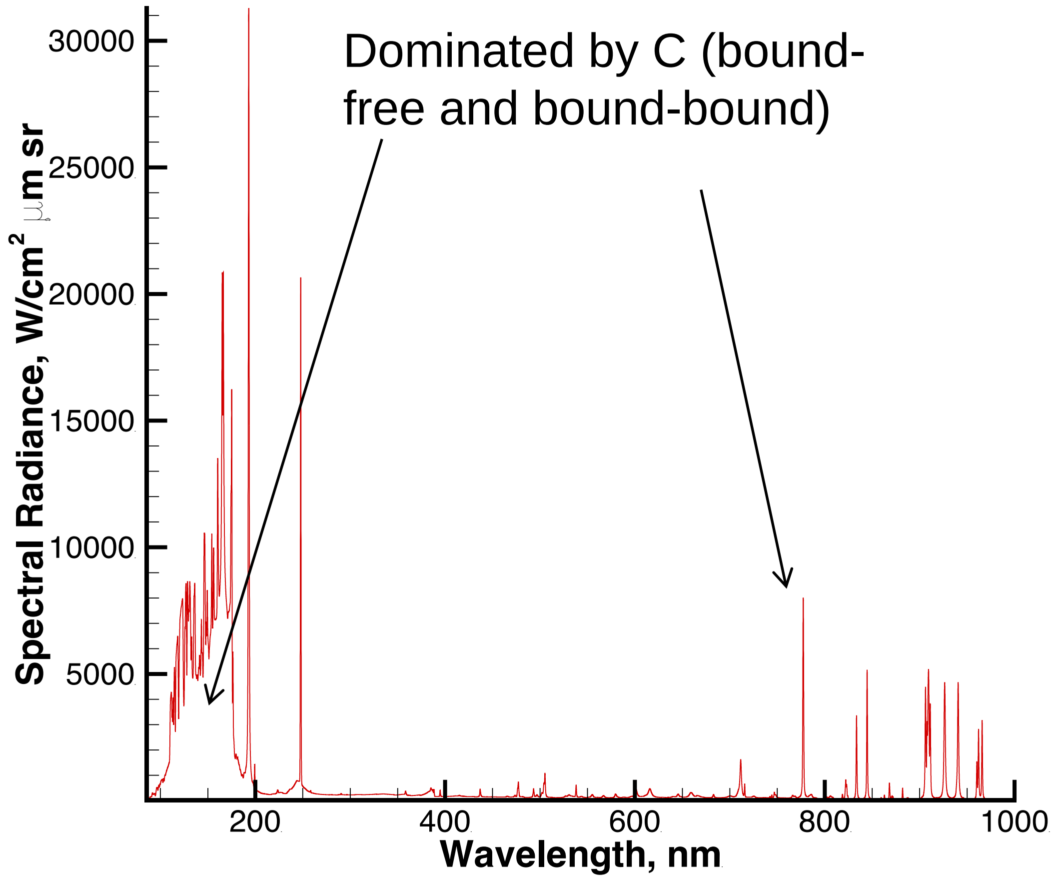
Entry Systems and Technology Division



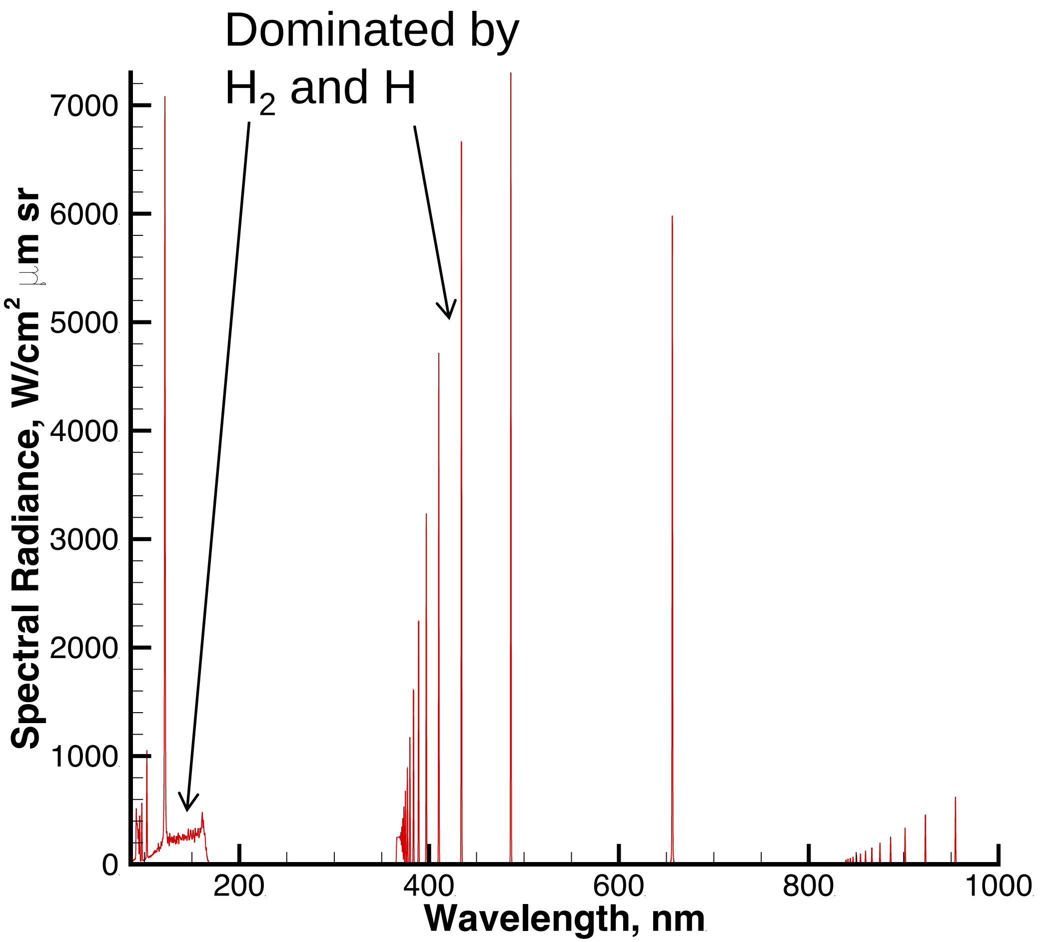
Titan Test Case



Venus Test Case



Saturn Test Case



Usage/Recommendation Notes

- Using CFD as input to NEQAIR
  - NEQAIR's best practice is to assume Te = Tv. If the CFD used to calculate the flowfield as input for NEQAIR assumes Te = Tt, erroneously large numbers can occur for high speed entry radiation. It is best practice for NEQAIR, to run CFD with Te = Tv.
- Grid type
  - Grid type 1 should be used as default. 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.
- 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. 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.

Usage/Recommendation Notes

- 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.
- Parsing CFD 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.

Updates to NEQAIR v13.2

- Mechanics of QSS have been updated.
- QSS now for CO 4th Positive, CN Violet.
- QSS updated for O_2 Schumann Runge.
- Mid-wave IR for CO_2 from CDSD database
- TOPBase data now used for continuum radiation.
- Atomic line list updated to NIST 5.0
- CO 4th Positive database updated to that of da Silva.
- More robust generation of EHL Files (files used for molecular radiation calculations).
- Pre-dissociation rates added for O_2 and NO,
- Radiance as a function of distance behind the shock data now output as LOS.out .
- Indexing of NEQAIR simplified, as a consequence fixed a bug for calculating the widths as ionization potential is correctly found.
- Scan process made more robust.

Updates to NEQAIR v14.0

- Parallel evaluation of different line of sight points - approximately 40x faster than v13.2 for test cases (speed up depends on number of points in LOS).
- Identifies and matches states assigned in lines and levels between QSS and TOPBase.
- More accurate tangent slab/spherical cap approximation.
- Saha distribution option for atomic excited states.
- Controlling temperatures changed for reverse reaction rates/equilibration in QSS – more consistent with CFD.
- Improved internal memory management.
- Checks for run-away answers based on inconsistencies with CFD Te input.
- Intensity.in can be specified (applies a defined spectral intensity at the first line of sight point).
- Emissivity.in can be specified (applies emissivity at final point in the line of sight e.g. emissivity of the TPS).
- 2-D output can be specified.
- Non-local ‘escape factor’ calculation can be performed for atoms.
- Option to calculate radiance in a shock tube orientation (i.e. normal to the flow direction).

How To Get the Code

- NEQAIR is no longer ITAR.
- NEQAIR is now EAR (export controlled).
- Anyone who works for an organization who has a contract with the United States government is allowed access to the code, provided that NEQAIR is relevant to the contracted work.
- To obtain the latest version of the code, v14.0, email two people:
  - Aaron Brandis: aaron.m.brandis@nasa.gov (NEQAIR PI)
  - Kim Chrestenson: kim.l.chrestenson@nasa.gov (Software Release Coordinator)
- Kim will then send you the latest Software Usage Agreement (SUA).
- Once she receives the signed SUA, she will inform me to send the source code, databases, test cases and an up-to-date user's manual.