# OH Model – overview

- Use MSIS to calculate the background data---z, N2, O2, O, H, Temp, Total numdens, Total massdens in cgs units
- Make a new folder for the new output files to go into eg. Test
- Copy the MSIS file into the new folder (alter file to include only altitudes wanted).
- Have the compatible NO.txt file in the same directory as the MSIS file (i.e., the NO over the same altitude range as MSIS)
- In Matlab, use addpath to set the path to the main Model top directory (that contains file AllA.m)
  Note, AllA sets the paths as to where to find the Einstein and rate coefficients to be used. These may have to be changed for your system.
- In Matlab, change to the folder containing the MSIS data (e.g. Test)
- Run AllA('msis.txt') in Matlab to calculate the rates and transition probabilities
- Run Meinel(adj), where adj is the value you wish to scale MSIS atomic oxygen by, to get the OH(v') densities and Iv'v" band intensities
- Run OHConc to get a graph of all OH v' concentrations
- Run IntensityGraph to get a graph of ν' intensity bands against altitude
- Run BandsGraphs('I9.txt') etc. to get a graph of all bands within a level

Note, AllA (11 is LL as in ALLA) sets the paths as to where to find the Einstein and rate coefficients to be used.

| Function | Example | Description | Input | File(s) needed | File(s) produced |
|---|---|---|---|---|---|
| AllA | AllA('MSIS.txt') | Calculates Einstein coefficients at temperatures of interest | MSIS file | MSIS.txt<br>NO.txt | A1.txt to A9.txt<br>rates1.txt to rates9.txt<br>background.txt |
| Meinel | Meinel(1) | Calculates the intensity bands of each v' to v'' level | Adjustment factor for MSIS [O] | A1.txt to A9.txt<br>rates1.txt to rates9.txt<br>background.txt | I1.txt to I9.txt<br>OH.txt<br>O3.txt<br>inttable.txt<br>Temp.txt |

Table 1

| Function | Graph produced |
|---|---|
| Ohconc | OH concentrations for each n' band vs altitude |
| Bandsgraphs('Ix.txt') | Intensity bands for all ν' to ν'' transitions (dependent on input) vs altitude |
| IntensityGraph | Intensity bands for ν'=1 to 9 vs altitude |

Table 2

CD to the directory labelled with your case (“case”)
Put the model input file into this directory
ALLA(‘model input file.txt’)

| File | Description | Format (column headings) | Units | Produced by |
|---|---|---|---|---|
| Inputs | | | | |
| MSIS.txt | MSIS background atmosphere file | z, N2, O2, O, H, T, numdens, massdens | km, molecules $cm^{-3}$, K | MSIS model<br>In case directory |
| NO.txt | NO mixing ratio | z, NO | Mixing ratio | User<br>In case directory or main model directory |
| v’v’’to’v’’’.txt | Transition probabilities | v' v" J' P1 Q1 R1 P2 Q2 R2 E1 E2 | $s^{-1}$ | User<br>In directory specified in ALLA.m |
| | | | | |
| Outputs | | | | All in case directory |
| A1.txt to A9.txt | Einstein coefficients | Temp, A98, A97, A96, A95, A94, A9 equivalent for A8 etc. | $s^{-1}$ | AllA(Av and Av1) |
| rates1.txt to rates9.txt | Rate constants for each v’ level | Temp, k1, k2a, k2b, k3, k4a, k4b,k5,k6 | K, $cm^3$ $s^{-1}$ | AllA(Constants) |
| background.txt | Background atmosphere concentrations | z,Temp,N2,O2,O,H,M,NO,CO2 | km, K, molecules $cm^{-3}$ | AllA(Constants) |
| I1.txt to I9.txt | Intensity of emission bands | I98, I97, I96, I95, I94, I9 | photons $cm^{-3}$ $s^{-1}$ $sphere^{-1}$ | Meinel |
| OH.txt | Table of [OH] for each level | OH9 to OH1 | molecules $cm^{-3}$ | Meinel |
| O3.txt | Table of [O3] profile | O3 | molecules $cm^{-3}$ | Meinel |
| Inttable.txt | Table of intensity levels for each tranistition | See Table 4 for format | kiloRayleighs | Meinel(raylightable) |
| Temp.txt | Table of Temperatures for each v’ band | v’, Temperature | K | Meinel(TempCalc) |

Table 3

| | | | | | |
|---|---|---|---|---|---|
| I1 | I10 | 0 | 0 | 0 | 0 |
| I2 | I20 | I21 | 0 | 0 | 0 |
| I3 | I30 | I31 | I32 | 0 | 0 |
| I4 | I40 | I41 | I42 | I43 | 0 |
| I5 | I50 | I51 | I52 | I53 | I54 |
| I6 | I61 | I62 | I63 | I64 | I65 |
| I7 | I72 | I73 | I74 | I75 | I76 |
| I8 | I83 | I84 | I85 | I86 | I87 |
| I9 | I94 | I95 | I96 | I97 | I98 |

Table 4

A model was produced to investigate various parameters affecting the vibrationally excited OH in the nightglow, specifically how Solar Proton Events it. The various reactions contributing to the production and loss of OH are given by reactions 1, 4, 5a and 5b shown in Table 1, steady state conditions where assumed. Reaction 1 is the major source of OH, the reaction populates only the ν' states from 9 to 6, according to the branching ratios given by Klenerman (1997). Reactions 5a and 5b are cascade reactions, they are the major source of OH in the lower ν' levels (see Table 2). Einstein A co-efficients were calculated from Mies (1974) at temperatures corresponding to the altitudes used. An MSIS background atmosphere was used to provide concentrations for all species, except NO, $CO_2$ and $O_3$, at1km altitude intervals between 75km and 125km. The ozone concentration was produced using reactions 2a, 2b, 3 and 6. The $CO_2$ concentration profile was interpolated from Kostsov (2002). The NO profile was initially set to zero.

| | Reaction | Rate Constant ($cm^3\ s^{-1}$) | Reference |
|---|---|---|---|
| 1 | H + O3 → HO* + O2<br>$6 \le \nu' \le 9$ | $k_1 = 1.4\times10^{-10}\exp(-470/T)$<br>$k_{1\nu}$ See Table 2 | Sander et al. (2006) |
| 2a | $O + O_2 + N_2 \rightarrow O_3 + N_2$ | $k_{2a} = 5.6\times10^{-34}(T/300)^{-2.6}$ | IUPAC Gas Kin. Dat. Ev. (2003) |
| 2b | $O + O_2 + O_2 \rightarrow O_3 + O_2$ | $k_{2b} = 6.0\times10^{-34}(T/300)^{-2.6}$ | IUPAC Gas Kin. Dat. Ev. (2003) |
| 3 | $NO + O_3 \rightarrow NO_2 + O_2$ | $k_3 = 1.4\times10^{-12}\exp(-1310/T)$ | IUPAC Gas Kin. Dat. Ev. (2003) |
| 4 | $OH_{\nu'}^* + O \rightarrow H + O_2$ | See Table 2 | Lopez-Moreno (1987) |
| 5a | $OH_{\nu'}^* + O_2 \rightarrow OH_{\nu'-1}^* + O_2$ | See Table 2 | See Table 2 |
| 5b | $OH_{\nu'}^* + CO_2 \rightarrow OH_{\nu'-1}^* + CO_2$ | See Table 2 | See Table 2 |
| 6 | $O + O_3 \rightarrow O_2 + O_2$ | $k_6 = 8.0\times10^{-12}\exp(-2060/T)$ | Sander et al. (2006) |

Table 1

| ν' | $\alpha_\nu = \frac{k_{1\nu}}{k_1}$ * | $k_4$ ($cm^3\ s^{-1}$) | $k_{5a}$ ($cm^3\ s^{-1}$) | $k_{5b}$ ($cm^3\ s^{-1}$) | Reference for $k_{5a}$ and $k_{5b}$ |
|---|---|---|---|---|---|
| 1 | -- | $9.80\times10^{-11}$ | $1.30\times10^{-13}$ | $1.80\times10^{-13}$ | a |
| 2 | -- | $8.60\times10^{-11}$ | $2.70\times10^{-13}$ | $4.80\times10^{-13}$ | a |
| 3 | -- | $7.40\times10^{-11}$ | $5.20\times10^{-13}$ | $1.40\times10^{-12}$ | a |
| 4 | -- | $6.20\times10^{-11}$ | $8.80\times10^{-13}$ | $2.80\times10^{-12}$ | a |
| 5 | -- | $5.00\times10^{-11}$ | $1.70\times10^{-12}$ | $9.00\times10^{-12}$ | e |
| 6 | 0.09 | $3.80\times10^{-11}$ | $3.00\times10^{-12}$ | $2.80\times10^{-11}$ | e |
| 7 | 0.19 | $2.60\times10^{-11}$ | $7.00\times10^{-12}$ | $6.70\times10^{-11}$ | b |
| 8 | 0.28 | $1.40\times10^{-11}$ | $8.00\times10^{-12}$ | $6.40\times10^{-11}$ | c |
| 9 | 0.44 | $2.00\times10^{-12}$ | $1.70\times10^{-11}$ | $5.70\times10^{-11}$ | d |
| 10 | -- | -- | $1.50\times10^{-11}$ | $1.86\times10^{-11}$ | c |
| 11 | -- | -- | $2.79\times10^{-11}$ | $1.90\times10^{-11}$ | c |

* Klenerman and Smith (1987)

a. Dodd (1991)
b. Knutsen (1996)
c. Dyer (1996)
d. Chalamala (1993)
e. Extrapolated from the rest of the data

References:


Sander, S. P., et al. (2006), Chemical kinetics and photochemical data for use in stratospheric modeling, Evaluation number 15, JPL Publ.

Klenerman, D and I. W. M. Smith, Infrared chemiluminescence studies using a SISAM spectrometer, [J. Chem. Soc. Faraday Trans. 2, 83, 339-241, 1997]

Evaluated kinetic and photochemical data for atmospheric chemistry: part 1 – gas phase reaction of $O_x$, $HO_x$, $NO_x$, and $SO_x$ species
R. Atkinson, D. L. Baulch, R. A. Cox, J. N. Crowley, R. F. Hampson, R. G. Hynes, M. E. Jenkin, M. J. Rossi, and J. Troe
Atmos. Chem. Phys. Discuss., 3, 6179-6699, 2003

Lopez-Moreno J.J., Rodrigo R., Moreno F., Lopez-Puertas M., Molina A., Altitude distribution of vibrationally excited states of atmospheric hydroxyl at levels $\nu$=2 to $\nu$=7, [Planet. Space Sci. 35 (8), 1029-1038, 1987]

Dodd J.A., Lipson S.J. and Blumberg W.A.M, Formation and vibration relaxation of $OH(X^2\Pi_i,\nu)$ by $O_2$ and $CO_2$, [J. Chem. Phys. 95 (8), 5752-5762 (1991)]

Knutsen K., Dyer M.J., Copeland R.A., Collisional removal of $OH(X^2\Pi_i,\nu=7)$ by $O_2$, $N_2$, $CO_2$ and $N_2O$, [J. Chem. Phys. 104 (15), 5798-5802 (1996)]

Dyer M.J., Knutsen K., Copeland R.A., Energy transfer in the ground state of OH: Measurements of OH($\nu$=8,10,11) removal, [J. Chem. Phys. 107 (19), 7809-7815 (1996)]

Chalamala B.R., Copeland R.A., Collision dynamics of $OH(X^2\Pi,\nu=9$ [J. Chem. Phys. 99 (8), 5807-5811 (1993)]

Kostsov V. S. and Timofeyev, Yu. M., Mesospheric Carbon Dioxide Content as determined from the CRISTA-1 experimental data [Izvestiya Atmospheric And Oceanic Physics 39 (3): 322-332 (2003)]

Mies, F. H., Calculated Vibration Transistion probabilities of OH(X2p), [J. Mol. Spec., 53, 150-188 (1974)]

Turnbull, D. N. and Lowe, R. P., New hydroxyl Transistion probabilities and their importance in airglow studies, [Plant. Space Sci., 37, 6, 723-738 (1989)]

Langhoff, S. R., Werner, H.-J. and Rosmus, P., Theoretical Transistion probabilities for the OH Meinel System, [J. Mol. Spec.,118, 507-529 (1986)]