Exceptional service in the national interest

SAND2015-1056PE

Sandia National Laboratories

The Aurora

Electron Transport in the Upper Atmosphere

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U.S. DEPARTMENT OF ENERGY NNSA

Outline

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Proposed Research

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- Model the physics of electron transport through the earth's atmosphere
- Numerically solve a transport equation governing this process
- Input would be an assumed electron distribution from a solar event
- Output would contain:
  1. Rates for every modeled electron reaction
  2. Energy deposition in the atmosphere
  3. Conservation of energy check
- Compare output of the solution to real atmospheric data

Importance of the Aurora

Scientific perspective:

- Help understand and interpret the observed energetic particle spectra
- Help explain the interactions between the thermosphere, ionosphere, and magnetosphere
- Better understand the heating mechanism in the upper atmosphere

http://en.wikipedia.org/wiki/Aurora

Importance of the Aurora

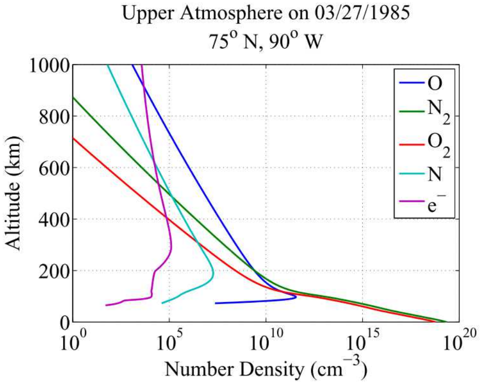
Sandia's perspective:

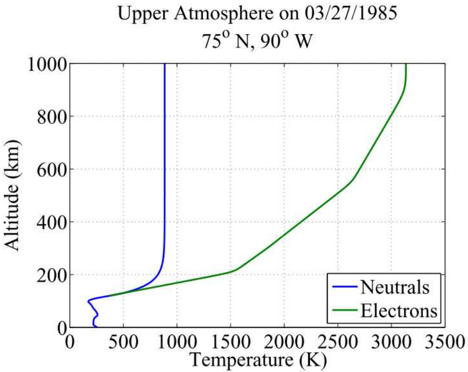
- Sandia's missions include monitoring the Limited Test Ban Treaty of 1963
- Want to model the emission of light from the upper atmosphere for a nuclear detonation (NUDET)
- Some of the effects of the aurora are the same as those for a NUDET

Courtesy of Sandia National Laboratories

Definition of the Upper Atmosphere

- Thermosphere and ionosphere
- Altitudes between $\sim 85 - 1000$ km





Calculated using codes MSIS-E-90 and IR

Outline

Cause of the Aurora

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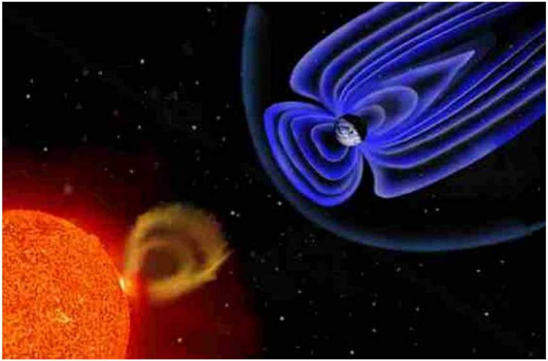
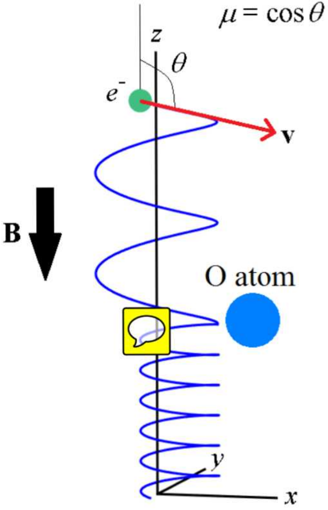
- Solar event sends out charged particles
- Solar particles scatter off atmospheric particles
- Scattering imparts energy to atmospheric particles
- Atmospheric particles release energy in the form of light



http://www.ecofriend.com/researchers-plan-to-harvest-solar-winds-for-renewable-energy.html

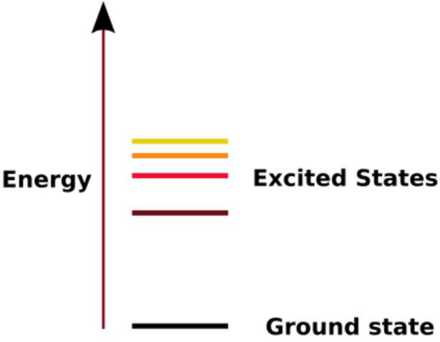
Electron Motion and Scattering

- Electrons travel in helical paths about the magnetic field lines
- Electrons have a chance to be scattered when they encounter atmospheric particles
- Scattering can:
    1. Change the direction θ of the incident electron
    2. Impart energy to the atmospheric particle – incident electron loses energy



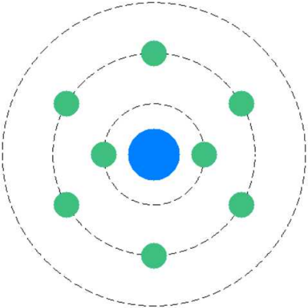
Atomic and Molecular States

- An atom or molecule has a certain configuration of electrons
- The configuration gives the atom or molecule a specific amount of internal energy
- An atom or molecule wants to have the lowest internal energy possible – the ground state
- All other states are called excited states



http://en.wikipedia.org/wiki/Energy_level

An Illustration of Excitation Scattering



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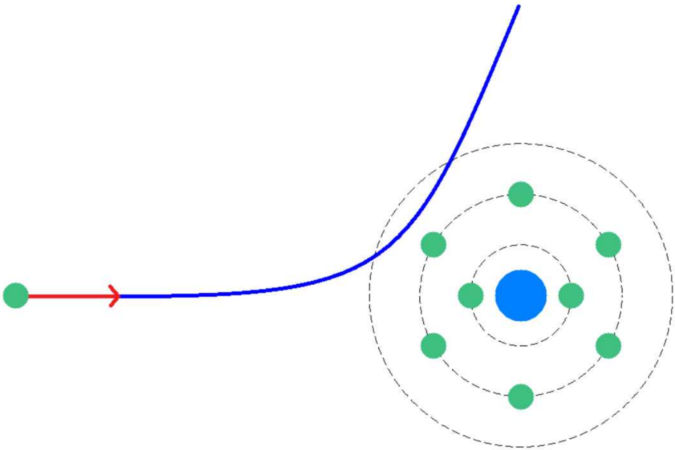

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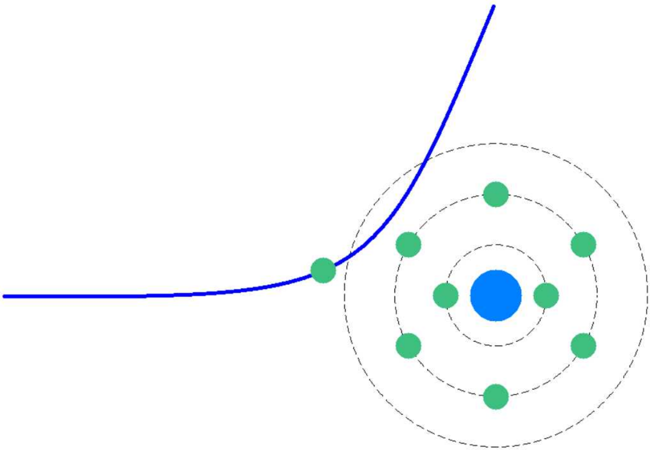

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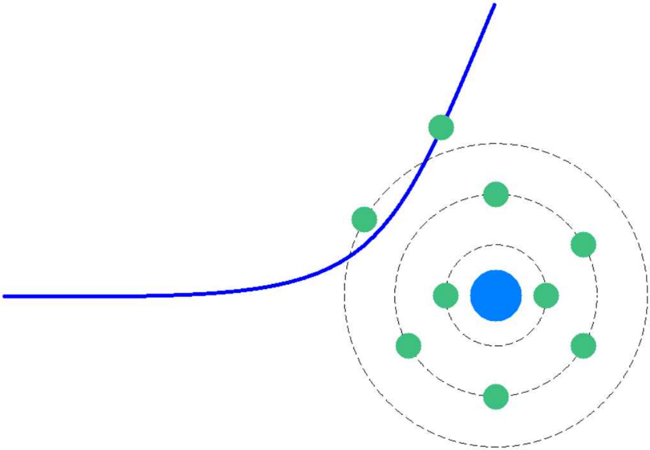

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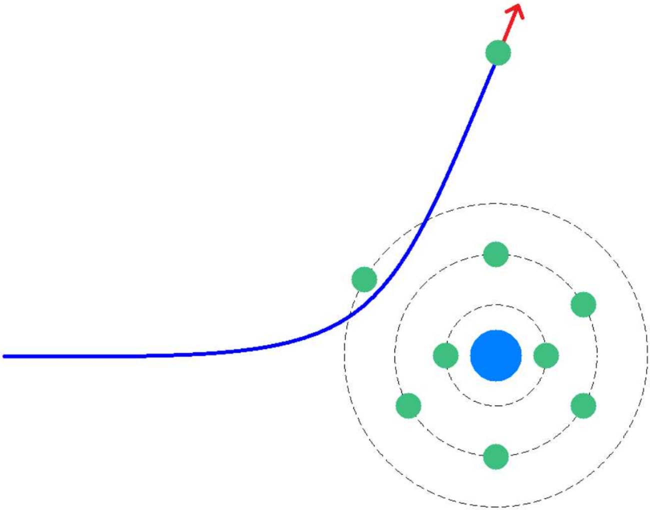

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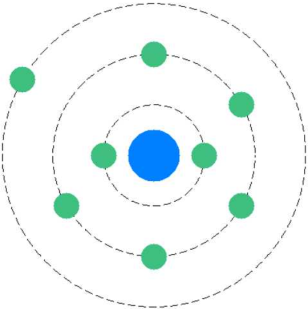

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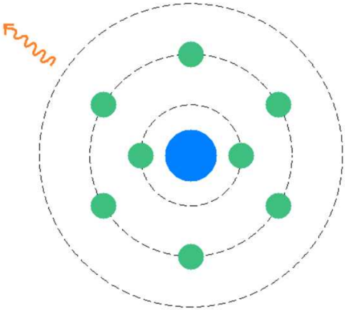
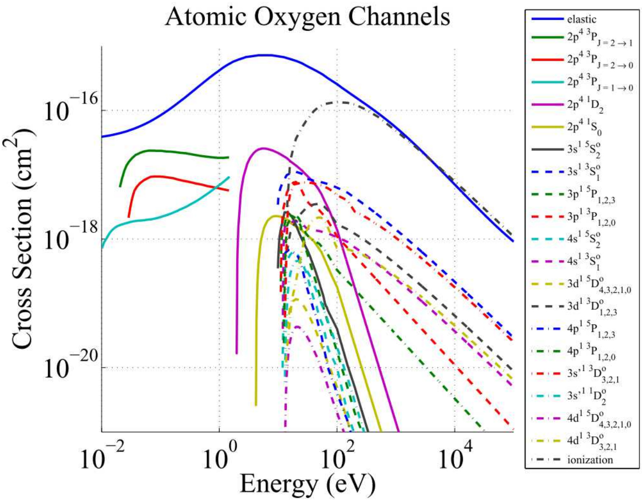


Scattering is Governed by Cross Sections

- Scattering is a probabilistic event
- Probabilities are governed by hypothetical areas called cross sections
- Cross sections depend on incident electron energy



Outline

Electron Intensity and Transport Assumptions

- Electron intensity (cm^{-2} s^{-1} eV^{-1} sr^{-1}) is a quantity that allows us to calculate quantities of interest (scattering rates and energy deposition)
- An equation for electron intensity can be derived from the continuity equation
- Equation assumes:
    1. Steady state
    2. Atmosphere is horizontally stratified
    3. Earth's magnetic field is uniform and vertical
    4. Atmospheric particles are at rest
    5. Electron intensity is azimuthally isotropic about the magnetic field lines

Electron Transport Equation

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Equation

$$\mu \frac{\partial I}{\partial z} - n_e(z) \frac{\partial}{\partial E}(LI) = Q(z,E,\mu) - \sum_{\substack{\text{species} \\ \xi}} n_\xi(z) \sigma_\xi^{\text{tot}}(E) I(z,E,\mu)$$

$$+ \sum_{\substack{\text{species} \\ \xi}} \sum_{\substack{\text{channel} \\ \eta}} \int_{E+W_\xi^\eta}^{E_{\max}} \int_{-1}^{1} S_\xi^\eta(z,E,E',\mu,\mu') I(z,E',\mu')\, d\mu' dE'$$

Boundary Conditions

$$I(z_{\text{top}}, E, \mu < 0) = I_{\text{top}}(E, \mu < 0)$$

$$I(z_{\text{bottom}}, E, \mu > 0) = 0$$

$$I(z, E > E_{\max}, \mu) = 0$$

Domain

$$z_{\text{bottom}} \leq z \leq z_{\text{top}}$$

$$0 \leq E \leq E_{\max}$$

$$-1 \leq \mu \leq 1$$

Electron Transport Equation

$$\mu \frac{\partial I}{\partial z} - n_e(z) \frac{\partial}{\partial E}(LI) = Q(z, E, \mu) - \sum_{\substack{\text{species} \\ \xi}} n_\xi(z) \sigma_\xi^{\text{tot}}(E) I(z, E, \mu)$$

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- Species = O, N_2, O_2, etc.

Electron Transport Equation

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- Species = O, N_2, O_2, etc.
- Channel = scattering reactions

Electron Transport Equation

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- Species = O, N_2, O_2, etc.
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- Electron intensity directional derivative

Electron Transport Equation

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- Species = O, N_2, O_2, etc.
- Channel = scattering reactions
- Electron intensity directional derivative
- Continuous slowing down of solar electrons

Electron Transport Equation

$$\mu \frac{\partial I}{\partial z} - n_e(z) \frac{\partial}{\partial E}(LI) = Q(z, E, \mu) - \sum_{\substack{\text{species} \\ \xi}} n_\xi(z) \sigma_\xi^{\text{tot}}(E) I(z, E, \mu)$$

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- Species = O, N_2, O_2, etc.
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- Internal source of electrons (photoionization)

Electron Transport Equation

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$$\mu \frac{\partial I}{\partial z} - n_e(z) \frac{\partial}{\partial E}(LI) = Q(z,E,\mu) - \sum_{\substack{\text{species} \\ \xi}} n_\xi(z)\sigma_\xi^{\text{tot}}(E) I(z,E,\mu)$$

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- Species = O, N_2, O_2, etc.
- Channel = scattering reactions
- Electron intensity directional derivative
- Continuous slowing down of solar electrons
- Internal source of electrons (photoionization)
- Out-scattering $\left(\sigma_\xi^{\text{tot}}(E) = \sum_\eta \sigma_\xi^\eta(E)\right)$

Electron Transport Equation

$$\mu\frac{\partial I}{\partial z} - n_e(z)\frac{\partial}{\partial E}(LI) = Q(z,E,\mu) - \sum_{\substack{\text{species}\\ \xi}} n_\xi(z)\sigma_\xi^{\text{tot}}(E)I(z,E,\mu)$$

$$+ \sum_{\substack{\text{species}\\ \xi}} \sum_{\substack{\text{channel}\\ \eta}} \int_{E+W_\xi^\eta}^{E_{\max}} \int_{-1}^{1} S_\xi^\eta(z,E,E',\mu,\mu')I(z,E',\mu')\,d\mu' dE'$$

- Species = O, N_2, O_2, etc.
- Channel = scattering reactions
- Electron intensity directional derivative
- Continuous slowing down of solar electrons
- Internal source of electrons (photoionization)
- Out-scattering $\left(\sigma_\xi^{\text{tot}}(E) = \sum_\eta \sigma_\xi^\eta(E)\right)$
- In-scattering

Boundary Conditions

- $I(z_{\text{top}}, E, \mu) = I_{\text{top}}(E, \mu)$ for $-1 \leq \mu \leq 0$
  1. $I_{\text{top}}(E, \mu < 0)$ depends on a particular solar event
  2. Some downward distribution must be assumed
- $I(z_{\text{bottom}}, E, \mu) = 0$ for $0 \leq \mu \leq 1$
  1. z_{bottom} is unknown (free boundary value problem)
  2. Part of the problem is to find z_{bottom}
  3. z_{bottom} is a function of energy
- $I(z, E, \mu) = 0$ for $E > E_{\text{max}}$
  1. E_{max} depends on a particular solar event
  2. Some maximum energy must be assumed

Outline

DISORT

- DISORT (**DIS**crete **O**rdinates **R**adiative **T**ransfer) was written in the 80's to solve photon transport problems
- It solves problems of the form

$$\mu \frac{\partial I}{\partial \tau} = Q(\tau, \mu) + I(\tau, \mu) - \omega(\tau) \int_{-1}^{1} P(\tau, \mu, \mu') I(\tau, \mu')\, d\mu'$$

  where $I(\tau_{\text{top}}, \mu < 0) = c$ and some reflectivity is specified for $I(\tau_{\text{bottom}}, \mu > 0)$
- Program only gives two choices for $Q(\tau, \mu)$

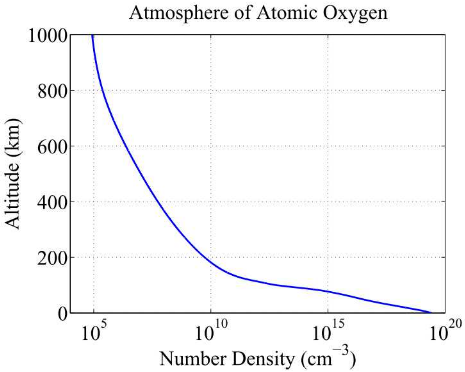
DISORT Applied to Electron Transport

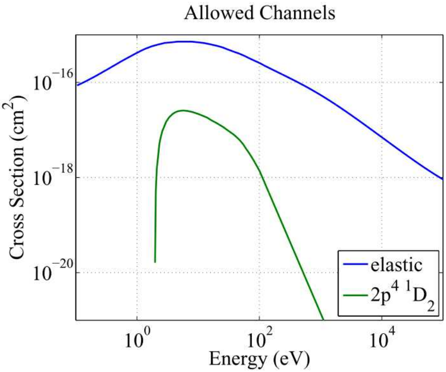
- DISORT was modified in the 90's so that it could be used for electron transport
- Electron transport terms not contained in DISORT's equation become a part of $Q(\tau, \mu)$
- Hold energy constant and invoke the modified DISORT program
- Works well for high energy electrons ($E > 5000$ eV)
- Very poor for low energy electrons ($E < 500$ eV)

Outline

Consider a Simplified Problem

- Consider a problem where
  1. The atmosphere is entirely atomic oxygen
  2. Only two channels exist – elastic scattering and scattering to the first excited state $^1D_2$
  3. There are no ambient electrons
  4. Photoionization does not take place





Simplified Electron Transport Equation

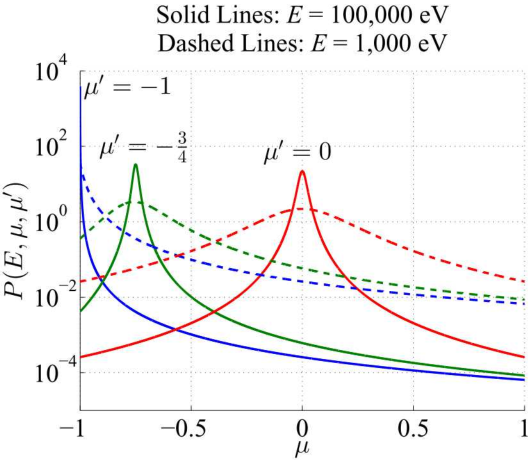
- For an elastic collision, no energy is transferred from the solar electron
- For an excitation collision, assume the solar electron is not deflected
- For an excitation collision, the energy transfer is exactly W

Simplified Equation

$$\mu \frac{\partial I}{\partial z} = - n(z)\sigma_{\text{tot}}(E) I(z, E, \mu) + n(z)\sigma_{\text{el}}(E) \int_{-1}^{1} P(E, \mu, \mu') I(z, E, \mu')\, d\mu' + \begin{cases} n(z)\sigma_{\text{ex}}(E+W) I(z, E+W, \mu), & E+W \leq E_{\text{max}} \\ 0, & E+W > E_{\text{max}} \end{cases}$$

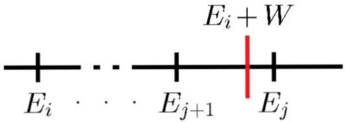
The Phase Function Causes Difficulty

- $P(E, \mu, \mu')$ is sharply peaked at $\mu = \mu'$ for large energies
- Causes quadrature approximation to require a prohibitively large number of points
- In practice we replace $P(E, \mu, \mu')$ by an expansion in a delta function and Legendre polynomials



Numerical Procedure

- Approximate the integral by a quadrature sum
- Discretize energy E_i for $i = 0, 1, \ldots, M$ such that $E_0 = E_{\max}$ and $E_M = 0$
- Evaluate the equation at $E = E_i$
- Approximate $I(z, E_i + W, \mu)$ by a linear interpolation in E



- Starting at $i = 0$, solve the boundary value problem using a 2-stage, 4th order implicit Runge-Kutta method
- Increment i and work downward in energy

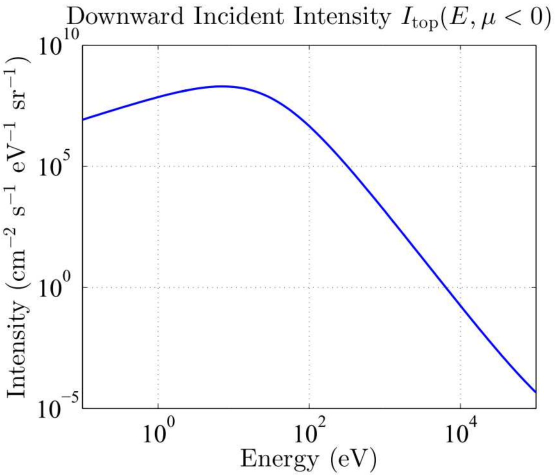
Free Boundary

- Physically, $I(z, E, \mu)$ must be non-negative
- Recall the boundary condition $I(z_{\text{bottom}}, E, \mu > 0) = 0$
- Picking z_{bottom} too low will result in the numerical solution going negative
- Picking z_{bottom} too high will result in an inaccurate solution
- Both cause the numerical solution to go to unstable as E decreases to 0
- My current work uses brute force to find z_{bottom}

Outline

An Assumed Downward Boundary Condition

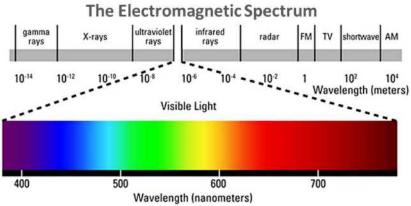
- Test transport algorithm with a sample problem
- Assume some downward distribution at the top of the atmosphere
- Assume downward incident intensity to be isotropic in pitch angle



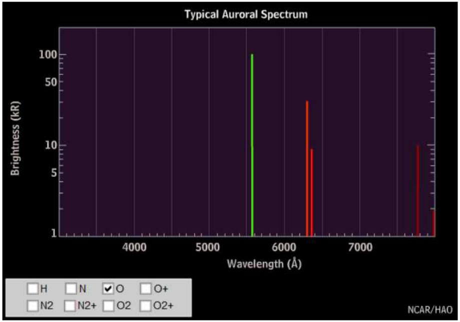
Show Movie of Solution

Oxygen Excitation

- $O(^1D_2)$ decays to either $O(^3P_2)$ or $O(^3P_1)$
- This gives the auroral "red doublet" with light at 630.2 nm and 636.6 nm



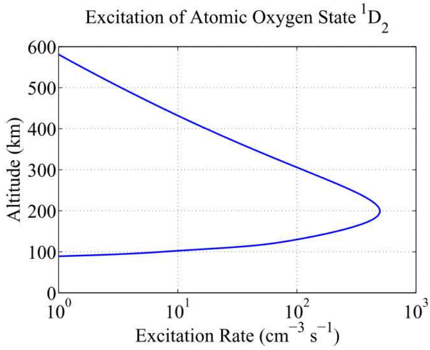
https://www.science3d.org/content/basic-principles-x-ray-tomography-x-rays

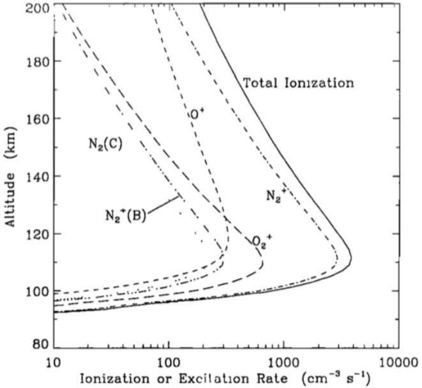


https://www.itp.uni-hannover.de/~zawischa/ITP/atoms.html

Excitation Rate Comparison

- Calculated excitation rate is qualitatively similar to excitation rates from a Monte Carlo simulation for a more realistic problem





[S. C. Solomon, *Geophys. Res. Lett.*, **20**, 186, 1993]

Conservation of Energy Check

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- There are two ways to calculate total energy deposition
- One way gives $\mathcal{E}_{\text{tot}} = 1.1785 \times 10^{10}$ eV/cm^2 s
- The other way gives $\mathcal{E}_{\text{tot}} = 1.1759 \times 10^{10}$ eV/cm^2 s
- The difference between the two is about 0.22%

$$\mathcal{E}_{\text{tot}} = 2\pi \sum_{\substack{\text{species} \\ \xi}} \sum_{\substack{\text{channel} \\ \eta}} W_\xi^\eta \int_{z_{\text{bottom}}}^{z_{\text{top}}} \int_{W_\xi^\eta}^{E_{\max}} \int_{-1}^{1} n_\xi(z) \sigma_\xi^\eta(E) I(z, E, \mu) \, d\mu \, dE \, dz$$

$$= 2\pi \left| \int_0^{E_{\max}} \int_{-1}^{1} I(z_{\text{top}}, E, \mu) \mu \, E \, d\mu \, dE \right|$$

Outline

Work That Needs to be Done

- Single species problem
  1. Derive a numerical method that includes a solution of the free boundary value problem
- Full problem
  1. Include principal reaction channels
  2. Include principal atmospheric species
  3. Include electron-electron interactions
- Auroral data
  1. Obtain auroral (electron intensity) data from rocket measurements
  2. Use measured intensity to supply boundary conditions
  3. Compare computed solution to the remainder of the measured intensity

Appendix: Quantities of Interest

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- Excitation/ionization rates (cm^{-3} s^{-1})

$$r_\xi^\eta(z) = 2\pi n_\xi(z) \int_{W_\xi^\eta}^{E_{\max}} \int_{-1}^{1} \sigma_\xi^\eta(E) I(z,E,\mu)\, d\mu\, dE$$

- Energy deposition rate (eV cm^{-3} s^{-1})

$$\mathcal{E}(z) = \sum_{\substack{\text{species}\\ \xi}} \sum_{\substack{\text{channel}\\ \eta}} W_\xi^\eta r_\xi^\eta(z)$$

- Total energy deposition (eV cm^{-2} s^{-1})

$$\mathcal{E}_{\text{tot}} = \int_{z_{\text{bottom}}}^{z_{\text{top}}} \mathcal{E}(z)\, dz = 2\pi \left| \int_0^{E_{\max}} \int_{-1}^{1} I(z_{\text{top}}, E, \mu)\mu\, E\, d\mu\, dE \right|$$