The Basics of Modeling the Thermosphere and Ionosphere
Now Available in 1D!

Aaron Ridley¹

¹Department of Atmospheric, Oceanic and Space Sciences
University of Michigan

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Outline

The Basics

Building an Atmosphere
  Hydrostatic
  Heating
  Conduction

Building an Ionosphere
  Chemistry
  Ion Advection
Basics of Modeling

- **Discretization** - taking a continuous series (in time and/or space) and breaking into discrete cells.
- **Assumptions** - what simplifications are made in order to allow the equations to be solved in a timely fashion?
- **Stability** - making sure the numerical method does not allow the solution to grow unbounded.
- **Boundary Conditions** - what happens at the edge of the simulation domain?
Discretization
Taylor Series Expansion - First Derivative

\[
T(z + \Delta z) = T(z) + \Delta z \frac{\delta T}{\delta z} + \frac{\Delta z^2}{2} \frac{\delta^2 T}{\delta z^2} + \ldots
\]

\[
T(z - \Delta z) = T(z) - \Delta z \frac{\delta T}{\delta z} + \frac{\Delta z^2}{2} \frac{\delta^2 T}{\delta z^2} - \ldots
\]

subtract...

\[
T(z + \Delta z) - T(z - \Delta z) = 2\Delta z \frac{\delta T}{\delta z}
\]

rearrange...

\[
\frac{\delta T}{\delta z} = \frac{T(z + \Delta z) - T(z - \Delta z)}{2\Delta z}
\]

Third order term is the first neglected. Said to be second order accurate.
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Summary

Discretization - 2
Taylor Series Expansion - Second Derivative

\[ T(z + \Delta z) = T(z) + \Delta z \frac{\delta T}{\delta z} + \frac{\Delta z^2}{2} \frac{\delta^2 T}{\delta z^2} + \ldots \]

\[ T(z - \Delta z) = T(z) - \Delta z \frac{\delta T}{\delta z} + \frac{\Delta z^2}{2} \frac{\delta^2 T}{\delta z^2} - \ldots \]

add together...

\[ T(z + \Delta z) + T(z - \Delta z) = 2T(z) + \Delta z^2 \frac{\delta^2 T}{\delta z^2} \]

rearrange...

\[ \frac{\delta^2 T}{\delta z^2} = \frac{T(z + \Delta z) + T(z - \Delta z) - 2T(z)}{\Delta z^2} \]

Third order term is the first neglected. Said to be second order accurate.
Discretization - 3
Solving on a grid:

- For a thermosphere, a spherical grid is typically used, with longitude, latitude and pressure (sometimes altitude). This can cause problems near the pole (models typically consider the pole a boundary.) New grids remove pole problem, but our field has yet to embrace these grids.

- For an ionosphere, a magnetic field-aligned grid is often used. This is complicated by the non-orthogonal nature of the magnetic field coordinate system. Assumptions are made.

- How to solve each direction (coupled or independently)? For the thermosphere, vertical is typically treated in a very different way than horizontal. For the ionosphere, along the field-line is treated differently than across the field-lines.

- As the equations of motion are solved for, the source terms must be added. How to treat these with respect to solving in the different directions?
Discretization - 4
Solving in time:

- Explicit - assume everything took place in last time step and the only place for the updated value is in the $\delta V/\delta t$ term. Relatively simple, but stability conditions are quite restrictive.

- Implicit - assume some things take place in the current time step, so the equations must be rearranged to solve for $V^{n+1}$. Usually adds significant complexity to the numerical scheme, but adds significant stability.

- Steady-state - assume $\delta V/\delta t = 0$. Solve equations. Strangely, this is applied in situations in which the value can change on a time scale much faster than the time-step. For example, the ion velocity is often assumed to be steady-state. Ion chemistry is sometimes assumed to be steady-state.
Assumptions
Every model has assumptions! For example:

- What equation set is the model solving? How is the model solving them? What is being neglected?
- What species are included? How is the chemistry solved?
- Parameterizations in things such as heating, cooling, viscosity, conduction, chemistry and diffusion. Collision, absorption, ionization cross sections, reaction rates,
- How are upper and lower boundaries treated? How is the pole or the open/closed field-line boundary treated?
- How are electrodynamics considered? How is the aurora specified? How is the magnetospheric electric field imposed? Is ion precipitation considered?
Stability
In reality, there are certain truths that cannot be broke (e.g., density and temperature cannot be negative). Within a model, these are not truths, and methods have to be employed to hold these truths.
Stability conditions are put on the model to try to ensure that the code does not violate these truths.
CFL Condition - make sure that material in a cell cannot pass all the way through the cell in one time-step. Given as the time-step must be lower than the cell width divided by the (total) velocity. This is not strictly needed for an implicit code.
Sharp Gradients
Low Order Scheme
Low order schemes are more stable, but more diffusive.

**Diffusive Solver**

![Graph showing the relationship between N (ions/cm^3) and x (meters). The graph shows a decrease in ion density as x increases.](image)
High Order Scheme
High order schemes capture more realistic features, but are less stable.
Boundary Conditions

Thing about boundary conditions in a couple ways:

1. You have gradients in the equations. How can you take a gradient at the bottom/top or side?

2. How will you keep the temperature/density/pressure from going to 0 or rising to infinity?

How to handle?

1. Set a value at the boundary. This will keep the values from becoming too large to too small.

2. Set a gradient at the boundary. (Can set the gradient to a specific value, like 0, or can set the gradient to the gradient above/below.) This is more liberal, but can cause stability problems.
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Outline

The Basics

Building an Atmosphere
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  Chemistry
  Ion Advection
Building an Atmosphere

\[ \frac{\partial P}{\partial z} + \rho g = 0 \]

\[ \frac{\partial P}{\partial z} = -\rho g \]

\[ \frac{\partial nT}{\partial z} = -\frac{nMg}{k} \]

\[ T \frac{\partial n}{\partial z} + n \frac{\partial T}{\partial z} = -\frac{nMg}{k} \]

\[ \frac{\partial n}{n} + \frac{\partial T}{T} = -\frac{Mg}{kT} \partial z \]

Note we make an assumption of changing temperatures on one side, but not on the other. Also \( g \) and \( M \) are assumed constant. \( P \) is pressure, \( z \) is altitude, \( \rho \) is mass density, \( g \) is gravity, \( n \) is number density, \( T \) is temperature, \( M \) is mass, and \( k \) is Boltzmann’s constant.
Building an Atmosphere - 2

\[
\frac{\partial n}{n} + \frac{\partial T}{T} = - \frac{Mg}{kT} \partial z
\]

\[
\ln \frac{n}{n_0} + \ln \frac{T}{T_0} = - \frac{\Delta z}{H}
\]

\[
n = \frac{n_0 T_0}{T} e^{-\frac{\Delta z}{H}}
\]

where \( H = \frac{kT}{Mg} \).
Building an Atmosphere - 3

\[ n = \frac{n_0 T_0}{T} e^{-\frac{\Delta z}{H}} \]

Now what?

1. Start at the bottom of the atmosphere with \( n_0 \) and \( T_0 \)
2. Calculate \( H \)
3. Step up by \( \Delta z \), calculating \( n \)
4. Set current \( n \) and \( T \) to \( n_0 \) and \( T_0 \)
5. Repeat 2-4 until top of atmosphere
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Summary
Single Species, Real Temperature, Better Formula

- From differential equation
- Iso-XX Atmosphere
- No Temperature Ratio
- With Temperature Ratio

Number Density (/m³)

Altitude (km)

Number Density (/m³)

Altitude (km)
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Summary

Three Species, Same Initial Density

![Graph showing the number density of different species versus altitude. The graph includes lines for [O2], [O], and [N2].]
Simplistically - hold $M$ to be the mean major mass (in the scale height) until the top of the homopause, then let the different masses diverge.
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Three Species, Realistic Initial Densities, Eddy Diffusion

Ta-Da! You have a realistic atmosphere in which the ratio of the different species is approximately correct.
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Heating an Atmosphere
Skipping a LOT of math....

\[ Q_{EUV} = \epsilon \sum_s \sum_\lambda n_s(z) \lambda I_\infty(\lambda) e^{-\tau} \sigma_s^a(\lambda) E(\lambda) \]

\[ \tau = \sec(\chi) \sum_s n_s(z) \sigma_s^a(\lambda) H_s \]

\( \epsilon \) is a heating efficiency (5% if you model the exothermic reactions explicitly, 35% if you don’t include chemistry), \( n_s(z) \) is the number density of species \( s \), \( \chi \) is the solar zenith angle, \( H_s \) is the scale height, \( \tau \) roughly the “optical depth”, \( E(\lambda) \) is the energy of the wavelength, \( I_\infty(\lambda) \) is the flux at the wavelength at infinity and \( \sigma_s^a(\lambda) \) is the absorption cross section.
Heating an Atmosphere - 2

\( I_\infty(\lambda) \) is the driven by the F\(_{10.7}\), and can be derived from the EUVAC model, which is specified in Table J.1 in Schunk and Nagy.

\( \sigma_s^a(\lambda) \) is the photoabsorption cross sections for the different species and are specified in Table J.2 in Schunk and Nagy.

You have to do a bunch of nested loops and everything is somewhat complicated. But, if you code everything right, you get an energy deposition profile....
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Heating the Atmosphere - 3

\[
\frac{\partial T}{\partial t} = \frac{Q_{EUV}}{\rho c_p}
\]

\(c_p\) is the specific heat of air at constant pressure (for a hydrostatic model), which is about 1500 J/kg/K. (Specifically it is \(C_p = V_{DoF} k/M\), which \(V_{DoF}\) is 5 for atoms and 7 for molecules.)
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Summary

Change of Temperature per Unit Time

\[ \frac{dT}{dt} \text{ (K/day)} \]

Altitude (km)

\[ \text{Altitude (km)} \]

\[ \frac{dT}{dt} \text{ (K/day)} \]

0 500 1000 1500

0 200 400 600
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Balancing the Heat
Heat in the thermosphere is conducted down to the lower thermosphere where it is dissipated by radiative cooling. Conduction is therefore very important. Here we will go through a bit of how to do conduction. First, steady-state:

\[- \frac{1}{\rho c_p} \frac{\partial}{\partial z} \lambda_n \frac{\partial T}{\partial z} = \frac{Q_{EUV}}{\rho c_p} \]

\[- \lambda_n \frac{\partial T}{\partial z} = Q_{EUV} \]

\[- \lambda_n \frac{\partial^2 T}{\partial z^2} = Q_{EUV} \]

\(\lambda_n\) is the thermal conductivity, which is given as \(\lambda_n = AT^S\), where \(A = 3.6 \times 10^{-4} \text{ W/m}\) and \(S = 0.75\) (simplistically).
Steady-State Conduction

\[
\frac{T(z + \Delta z) + T(z - \Delta z) - 2T(z)}{\Delta z^2} = -\frac{Q_{EUV}}{\lambda_n}
\]

\[
T(z - \Delta z) - 2T(z) + T(z + \Delta z) = -\frac{Q_{EUV} \Delta z^2}{\lambda_n}
\]

Look up “tri-diagonal solver” on wikipedia.

\[
a = 1 \\
b = -2 \\
c = 1 \\
d = -\frac{Q_{EUV} \Delta z^2}{\lambda_n}
\]

Boundary Conditions???
Non-Steady-State, Implicit Conduction

\[
\frac{\partial T}{\partial t} = \frac{Q_{EUV}}{\rho c_p} + \frac{1}{\rho c_p} \frac{\partial}{\partial z} \lambda_n \frac{\partial T}{\partial z}
\]

\[
\rho c_p \frac{\partial T}{\partial t} = Q_{EUV} + \left[ \frac{\partial \lambda_n}{\partial z} \frac{\partial T}{\partial z} + \lambda_n \frac{\partial^2 T}{\partial z^2} \right]
\]

use Taylor-series expansion...

\[
\frac{\rho c_p}{\Delta t} (T_{i+1} - T_{i-1}) = Q_{EUV} + \frac{\lambda_{i+1} - \lambda_{i-1}}{2\Delta z} \frac{T_{i+1} - T_{i-1}}{2\Delta z} + \lambda \frac{T_{i+1} + T_{i-1} - 2T_i}{\Delta z^2}
\]

note \(T^{n-1}\). Let \(\Delta \lambda = \lambda_{i+1} - \lambda_{i-1}\) do some math and rearrange....
Non-Steady-State, Implicit Conduction - 2

\[-\lambda T_{i+1} - \frac{1}{4} \Delta \lambda T_{i+1} + 2\lambda T_i + \frac{\rho c_p \Delta z^2}{\Delta t} T_i\]

\[-\lambda T_{i-1} + \frac{1}{4} \Delta \lambda T_{i-1} = \frac{\rho c_p \Delta z^2}{\Delta t} T_i^{n-1} + Q_{EUV} \Delta z^2\]

tri-diagonal solver....

\[a = 1 + \frac{\Delta \lambda}{4\lambda}\]

\[b = -2 - \frac{\rho c_p \Delta z^2}{\lambda \Delta t}\]

\[c = 1 - \frac{\Delta \lambda}{4\lambda}\]

\[d = -\frac{\Delta z^2}{\lambda} \left( \frac{\rho c_p}{\Delta t} T_i^{n-1} + Q_{EUV} \right)\]
Non-Steady-State, Implicit Conduction - 3
Boundary Conditions!
Top: $\partial T/\partial z = 0$, which means $T_{i+1} = T_i$, so

\[
\begin{align*}
    a &= 1 \\
    b &= -1 \\
    c &= 0 \\
    d &= 0
\end{align*}
\]

Bottom: $T=$Constant (say 200K), which means:

\[
\begin{align*}
    a &= 0 \\
    b &= -1 \\
    c &= 0 \\
    d &= -200
\end{align*}
\]
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Chemistry Basics

\[
\frac{\delta N}{\delta t} = S - L
\]

where \( N \) is the number density of the species, \( S \) represents the sources and \( L \) represents the losses. Losses almost always can be expressed as:

\[
L = R \times M \times N
\]

where \( R \) is the reaction rate, \( M \) is the density of the species it is reacting with and, once again, \( N \) is the number density of the species.
Steady-State Chemistry

\[ \frac{\delta N}{\delta t} = S - L \]

\[ 0 = S - L \]

\[ S = L \]

\[ S = R \times M \times N \]

\[ N = \frac{S}{R \times M} \]

This is quite stable, but can be very wrong in regions of slowly changing ion densities, such as in the F-region. This is perfect for the E-region, though. It is quite easy to implement in a simple environment, but can be much more complicated as non-linear terms are included (recombination, in which \( M \) can depend on \( N \)).
Explicit Time-Step Chemistry

\[
\frac{\delta N}{\delta t} = S - L
\]

\[
N - N^{i-1} \over \Delta t = S - R \times M \times N^{i-1}
\]

\[
N - N^{i-1} = \Delta t(S - R \times M \times N^{i-1})
\]

\[
N = N^{i-1} + \Delta t(S - R \times M \times N^{i-1})
\]

This is trivial to implement in almost all situations. BUT, it is the least stable, since the loss terms can become larger than the source terms and the density can quickly be driven to negative values. Subcycling can help with this, but not always.
Implicit Time-Step Chemistry

\[
\frac{\delta N}{\delta t} = S - L
\]

\[
\frac{N - N^{i-1}}{\Delta t} = S - R \times M \times N
\]

\[
N - N^{i-1} = \Delta t(S - R \times M \times N)
\]

\[
N = N^{i-1} + \Delta t(S - R \times M \times N)
\]

\[
N(1 + R \times M \times \Delta t) = N^{i-1} + S\Delta t)
\]

\[
N = \frac{N^{i-1} + S\Delta t}{1 + R \times M \times \Delta t}
\]

This is a relatively stable scheme and easier to implement than steady-state. In GITM, we have a blend between sub-cycling and a simplified implicit scheme that switches depending on the size of the loss term compared to the density.
Practical Chemistry

- Look back at $Q_{EUV}$ and substitute $\sigma_s^i \lambda$ instead of $\sigma_s^a \lambda$ (NOT IN $\tau$!!!). Now you have the ionization rates (i.e., source terms!).
- Look in Schunk and Nagy in Chapter 8 for a bunch of chemical equations.
- Write the sources and losses. Decide on a time scheme.
- Code.
- Run.
If we don’t have any ion advection, the F-region will just build and build.
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Super Simple Ion Advection

1. Take either upward or downward flow (i.e., $V_p = \max(V, 0)$, $V_m = \min(V, 0)$).

2. Take gradients in the upward and downward direction (i.e., $\Delta O_m^i = (O^i - O^{i-1})/\Delta z$ and $\Delta O_p^i = (O^{i+1} - O^i)/\Delta z$).

3. Calculate net change: $\Delta O = -\Delta t(\Delta O_p^i \times V_p + \Delta O_m^i \times V_m)$

4. $O^{N+1} = O + \Delta O$

This is first order, and is quite diffusive.
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Example Ionosphere \( V = -5 m/s \)

F-region peak is lower in altitude and density.
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Example Ionosphere $V = -10 \text{m/s}$

F-region peak is even lower in altitude and density.
Summary

- Building a simple, diffusive model is relatively easy.
- You have to understand the assumptions in the model to be able to study the physics that you really want to study.
- Hopefully you have learned a bit on how to build a simple 1D thermosphere and ionosphere!