Development of high-top (whole atmosphere) models

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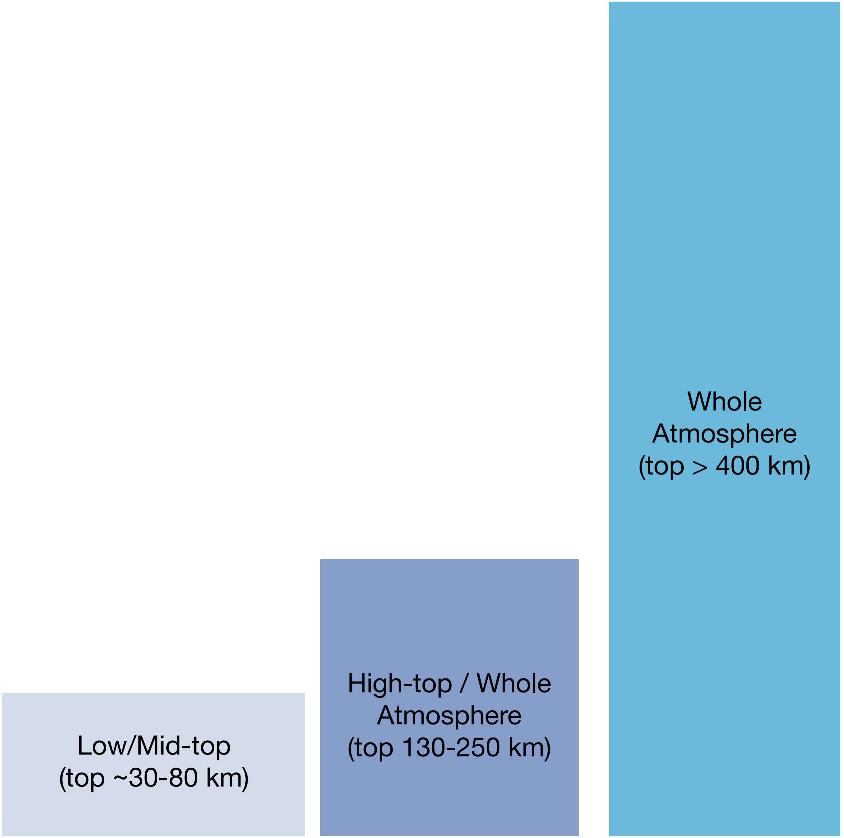
17 September 2024

This material is based upon work supported by the National Center for Atmospheric Research, which is a major facility sponsored by the National Science Foundation under Cooperative Agreement No. 1852977.



Low/Mid-top
(top ~30-80 km)

High-top / Whole
Atmosphere
(top 130-250 km)

Whole
Atmosphere
(top > 400 km)

Outline

- Why build a high-top atmosphere model?

- Developments needed for high-top models:
  - Heating and cooling processes
  - Gravity wave parameterizations
  - Molecular diffusion and viscosity
  - Ionospheric effects

- Active areas of development

Why build a high-top atmospheric model?

- Scientific understanding of the dynamics and chemistry of the mesosphere and lower thermosphere (i.e., fundamental understanding of Earth's atmosphere and space environment).
- Capture downward coupling effects that can influence climate/weather that require a well-resolved stratosphere-mesosphere (sudden stratosphere warmings, QBO, etc.).
- Simulate Solar influence on climate and weather.
- Incorporate effects of the troposphere-stratosphere on space environment.

Example application: Downward transport of nitrogen oxides (NO_x) into the stratosphere

Ratio of Observed NO_x to Climatology for SSW Winters

Downward transport of EPP (energetic particle precipitation) produced NO_x can lead to destruction of stratospheric ozone in polar winter.

Possible mechanism for solar influences on climate and weather.

(Randall et al., 2009, 2010)

Example application: Impact of lower atmosphere on space environment

Difference in satellite position after 24h at 200 km (left) and 400 km (right) when accounting for atmospheric tides propagating from the lower atmosphere

As low-Earth orbit becomes more crowded, accurate specification and forecasting of thermosphere mass density variations is becoming more important

(Leonard et al., 2012)

Example application: Impact of lower atmosphere on space environment

Ionosphere model w/ lower atmosphere variability

Ionosphere model w/ climatological winds

Observations

Accurately capturing the variability of the ionosphere, which effects communication and navigation signals, requires incorporating effects of the lower atmosphere

(McDonald et al., 2015)

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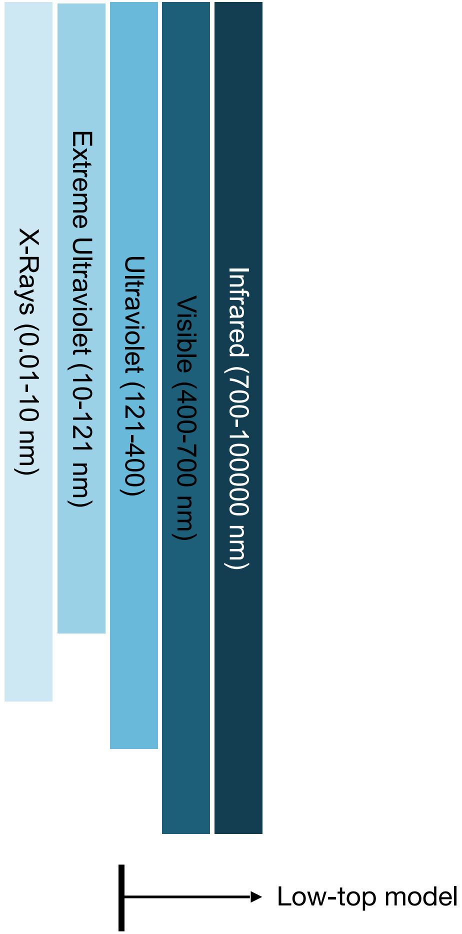
Whole atmosphere models need to account for a wider range of solar radiation inputs



X-Rays (0.01-10 nm)

Extreme Ultraviolet (10-121 nm)

Ultraviolet (121-400)

Visible (400-700 nm)

Infrared (700-100000 nm)

Low-top model

Solar EUV Radiation

- The thermosphere absorbs solar radiation at EUV wavelengths, ultimately leading to production of the ions and heating of the neutrals

- Solar radio flux at 10.7 cm (F10.7) is used as a proxy for EUV variations.

- Solar input in different wavelength bands is parameterized based on solar flux, typically using the EUVAC model of Richards et al. (1994)
    - Some models use a reduced set of 23 ‘Stan-bands’ (Solomon and Qian, 2005)

Solar EUV Energy Deposition (log$_{10}$(Wm^{-4})

Solar EUV variability over solar cycle and solar rotation

(Lean et al., 2003)

Solar EUV Radiation

- Based on a reference solar spectrum, the incident solar radiation at different wavelengths can be calculated.

- Using absorption cross sections and branching ratios, rates of photoionization, dissociative ionization, and dissociation can be obtained for the major thermosphere species (O, O_2, N_2)

(Richards et al., 1994)

Ionization of Neutral Particles

- Additional chemical reactions are necessary to incorporate the ionization of neutral particles as well as the ion-neutral interactions.

- Additional reactions are primarily related to the N^+, N_2^+, O^+, O_2^+, and NO^+.

Chemistry in the mesosphere and lower thermosphere (ionosphere D-region) can be significantly expanded for accurate representation of the chemistry, such as the effects of energetic particle precipitation and metal layers

(Verronen et al., 2016)

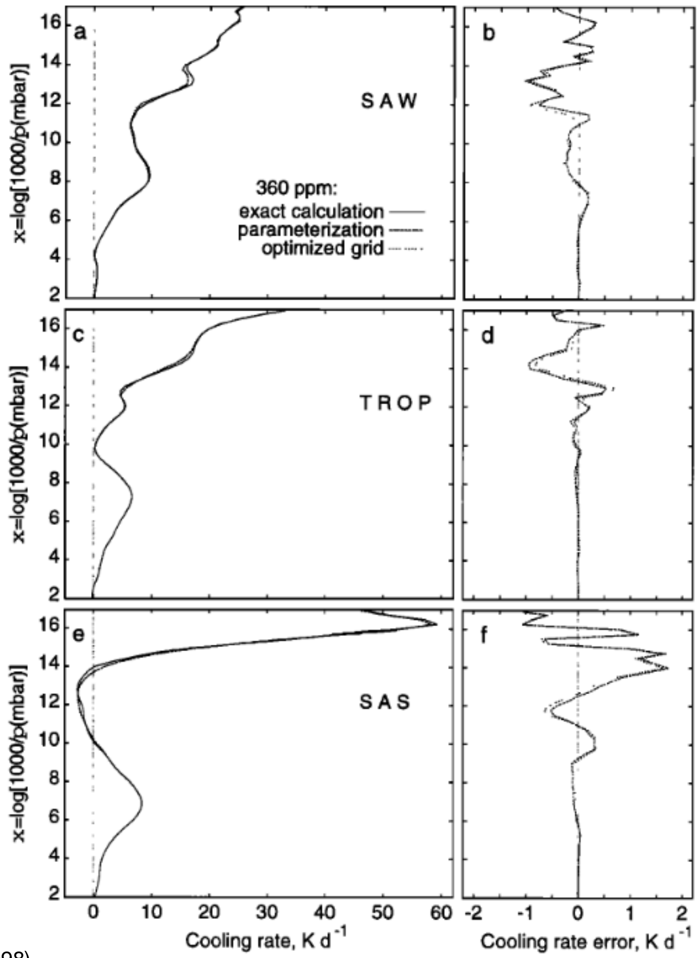
Modifications to longwave radiation schemes

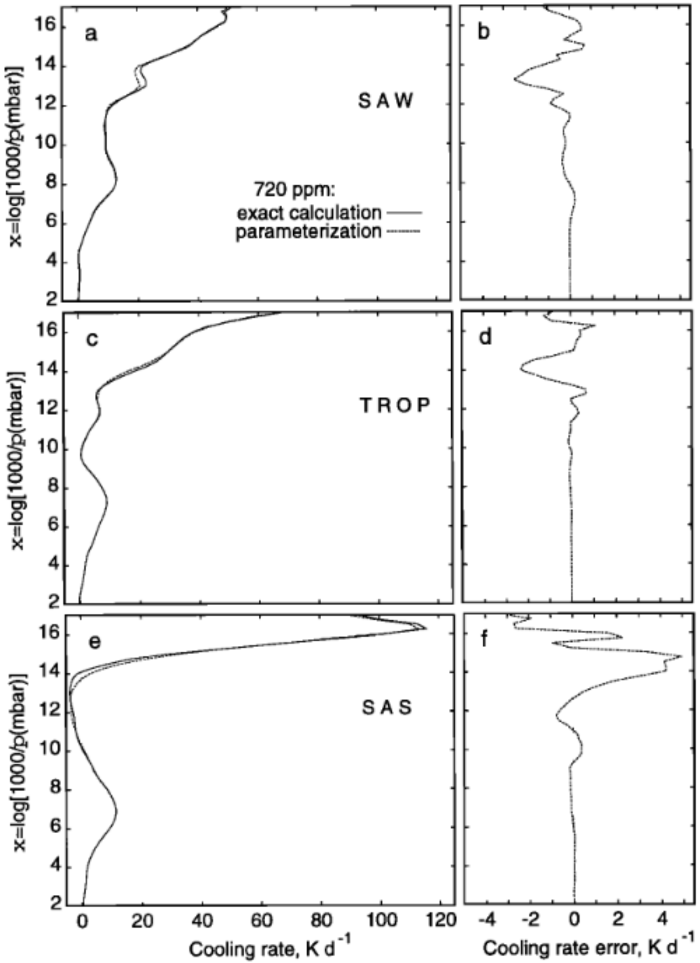
- Infrared radiative cooling by CO_2, O_3, and NO become significant above ~60-70 km.
- Modifications to the longwave radiation scheme are therefore required in order to accurately simulate the mesosphere and lower thermosphere.
- Non-local thermodynamic equilibrium (non-LTE) effects must also be considered about ~80 km.
- Most (all?) models use the formulations of Fomichev et al. (1998) and Fomichev and Blanchet (1995) for CO_2 and O_3.
- Kockarts (1980) provides a scheme for NO radiative cooling in the thermosphere.
- Transition region around ~60-70 km is used between the standard longwave radiation scheme and the Kockarts/Fomichev schemes.

Non-Local Thermodynamic Equilibrium

- Non-LTE conditions arise when the temperature of a molecule, determined by vibrational and rotational energy levels, becomes different from the temperature as defined by the velocity distribution of the molecules of a gas parcel.
- Largely depends on the mean rate of collisions, and thus non-LTE conditions become more important at higher altitudes
- Without accounting for non-LTE effects, CO_2 cooling would be > 100 K/day in the lower thermosphere

(Akmaev and Fomichev, 1998)





(Fomichev et al., 1998)

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Gravity Waves

- Gravity waves are essential for obtaining an accurate representation of the mesosphere and lower thermosphere due to their impact on the large-scale circulation as well as eddy diffusion of chemical species.

- Due to computational constraints, sub-grid scale gravity wave drag parameterizations remain an important component of high-top models.

- The impacts of non-orographic gravity waves is of primary importance to the mesosphere and lower thermosphere.

Aspects of Gravity Wave Drag Parameterizations

- Gravity wave drag parameterizations share common features:
  - Source (location, trigger, phase speed spectrum)
  - Wave growth (~$e^{Z/2H}$)
  - Wave saturation (i.e., breaking) and resultant momentum deposition and heating
  - Constituent transport

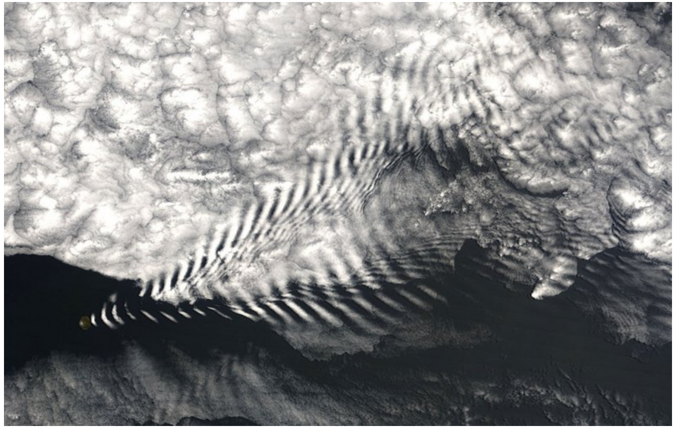
Gravity wave sources

- Gravity wave sources can be grouped into two categories: orographic and non-orographic

- Orographic gravity waves are related to flow over topography, and can be represented by relatively straightforward parameterizations.

- Non-orographic gravity waves arise from several sources, such as convection, jets, and fronts.

- Non-orographic gravity wave parameterizations vary widely across models in terms of complexity and treatment of the wave sources.



Non-orographic gravity waves

- Non-orographic gravity wave parameterizations rely on defining a momentum flux (τ) at a source region.

- A spectrum of waves is launched with different phase speeds (c) that can then be represented analytically using linearized equations (e.g., Lindzen, 1981).

- The most basic parameterizations assume a uniform source, such as:

- Basic non-orographic gravity wave drag parameterizations rely on uniform and/or basic variability (latitude and season) in the value of τ_b.

Non-orographic gravity waves

- More physically based non-orographic gravity wave parameterizations rely on defining a momentum source and phase speed spectra based on physical properties, such as convection or the location of fronts.
- Richter et al. (2010) uses a frontogenesis function to serve as a trigger of the initiation of gravity waves:
- Beres et al. (2005) also developed a gravity wave source parameterization that is dependent upon the model convection.
- Note that all gravity wave parameterizations involve a number of tunable parameters, including source altitude, amplitude, phase speeds, convective fraction, …

Orographic Gravity Waves

- Orographic gravity wave parameterizations consider the sub-grid scale orography for parameterizing the gravity wave source
- The parameterization of McFarlane (1987) is widely adopted:

Gravity Wave Saturation and Dissipation

- The wave amplitude grows with height due to the decrease in density, eventually reaching the point where it is unstable
- Once the instability criterion is reached, the wave amplitude no longer grows (wave saturation).
- This results in an additional momentum forcing and heating that is a major driver of the circulation in the middle atmosphere.

DJF Gravity Wave Drag
(in WACCM 3.5)

(Richter et al., 2010)

Gravity Wave Propagation

- Decrease in atmospheric density with height means that the wave amplitude grows as $e^{Z/2H}$ to conserve momentum

- Key assumptions for most gravity wave parameterizations:
  - Gravity waves propagate only in a vertical column
  - Propagation is instantaneous

(Sato et al., 2011)

Gravity Wave Impacts on Constituents

- Wave breaking produces an additional eddy diffusion, leading to an additional mixing of particles in the vertical direction.

- The eddy diffusion represents the vertical mixing that is unresolved by the model and is given by

  where Kzz is the eddy diffusion coefficient that is a product of the gravity wave parameterization:

- The eddy diffusion is further impacted by the Prandtl number that describes the ratio of eddy momentum flux to the eddy flux of chemical species.

Gravity Wave Impacts on Constituents

Pr = 4

Pr = 1

Both the Prandtl number and eddy diffusion coefficient have large uncertainties yet they significantly impact the constituent densities in the mesosphere and lower thermosphere.

(Smith-Johnsen et al., 2022)

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Molecular Diffusion and Viscosity

- Molecular diffusion begins to dominate above the mesopause, becoming more important than eddy diffusion.

- Molecular diffusion of individual species must therefore be considered in order to appropriately model the species distributions at high altitudes.

- The thermosphere is characterized by large viscosity and thermal conductivity, both of which must also be modified at high altitudes.

Vertical molecular diffusion

Vertical molecular diffusion for species (X_i) is given by:

where the diffusion coefficient and effective separation velocity are specified as (Banks and Kockarts, 1973):

Note that the above are only valid for species in a well mixed atmosphere or for minor species. In the thermosphere different treatment is needed for diffusion of the major species O, O_2, and N_2

Simulated CO_2 tendencies in WACCM (Smith et al., 2011)

ppmv/day

Molecular viscosity and thermal conductivity

- Both molecular viscosity and thermal conductivity have a large impact on the dynamics and temperature structure above ~100 km.

- To account for these effects, vertical diffusion of momentum and temperature are incorporated.

- Expressions for the viscosity (μ) and thermal conductivity (η) are often simplified as

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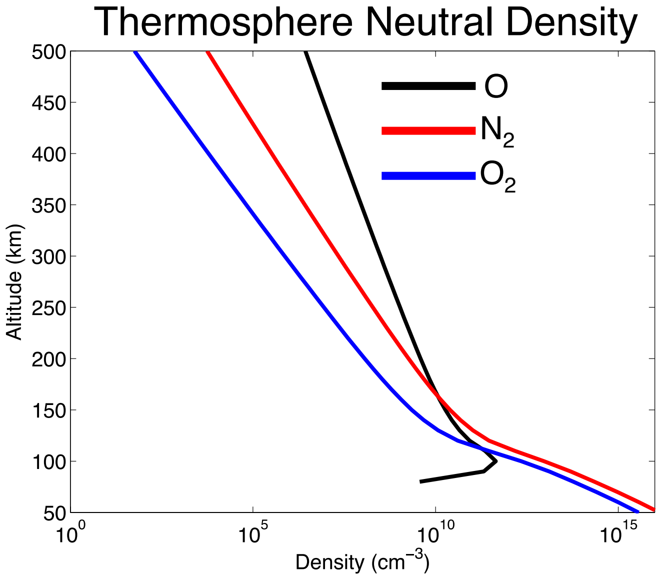
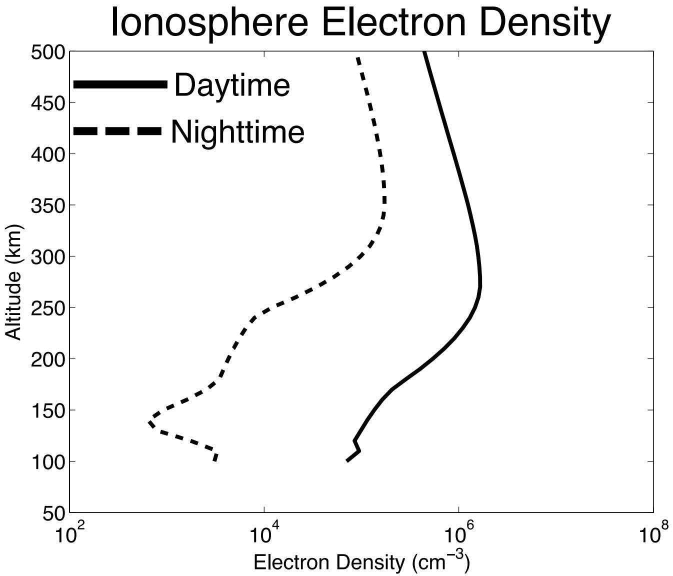
Above ~100 km solar ionization leads to the formation of the ionosphere, which influences the neutral dynamics





For models that don't explicitly solve for the ionosphere, a parameterized ion drag force is included through an additional tendency for the zonal and meridional winds

Ion drag parameterization

- Different parameterizations exist for the ion drag term, though they are all based on the fact that collisions between ions and neutrals imposes a forcing to the neutral gas.
- The ion-drag force is related to the ions being constrained to the magnetic field lines.
- Common parameterizations follow Hong and Lindzen (1976):

Ion drag

Lorenz force

Ion drag parameterization

- Lorenz term is only present at lower altitudes, where the collision frequency is much larger than the ion gyrofrequency.
- At higher altitudes the opposite is true, and the ions are constrained to the fields lines and induce a drag force on the neutrals.

(Hong and Lindzen, 1976)

Ion drag parameterization

- There are other formulations of the effects of the ionosphere on the neutral dynamics, but the physics of the interactions remain the same.

- Alternative ion drag parameterizations use different descriptions of the background ion and neutral densities which results in different parameterized ion drag.

- For example, CESM-WACCM adopts a slightly different formulation that is based on a more detailed treatment of the background ionosphere.

High Latitude / Auroral Processes

- There is significant additional energy input at high latitudes due to energetic particle precipitation and Joule heating.
- Particle precipitation can be specified (e.g., CMIP EPP) or parameterized based on the level of geomagnetic activity.
  - These effects are relevant for both heating as well as their effects on chemistry, such as EPP-NO_x
- Joule heating arises from the differential motion of plasma and neutrals:
- Joule heating can be a large (20 K/day) heat source at high latitudes.

Active areas of development (non-comprehensive list)

- Development of non-hydrostatic whole atmosphere models
- High-resolution capabilities, including nested grids
- Gravity wave parameterizations: non-vertical propagation, secondary waves, parameterizations for the thermosphere, scale awareness
- ML/AI
- …