The Vertical Structure of the Atmosphere

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Weather and Climate Seminar

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Outline

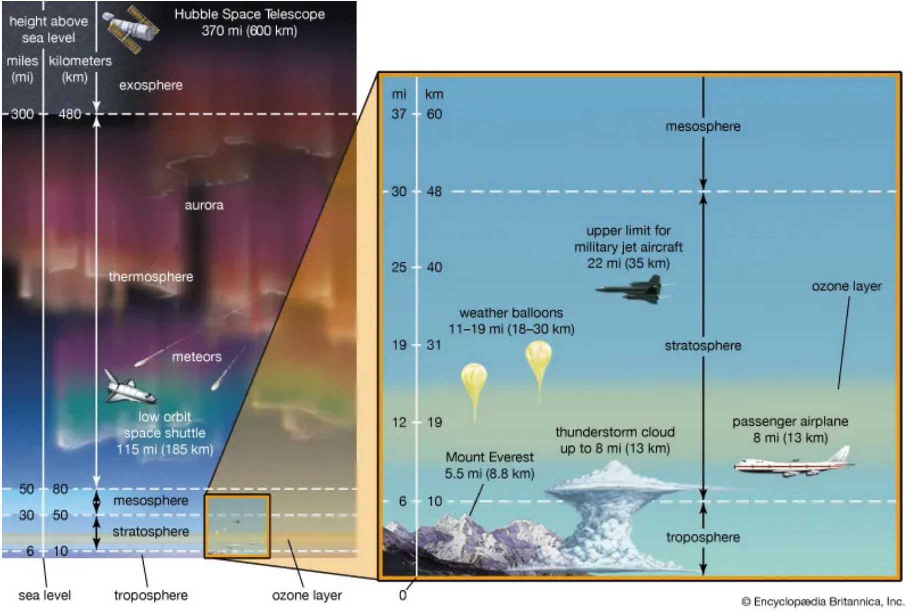
Introduction

Variation of the atmosphere, and the quantities we're looking at.

- Temperature
- Pressure
- Density

Briefly look at some quantum mechanical properties of Greenhouse gases that are responsible for this structure.

Structure of the atmosphere



The Temperature Profile

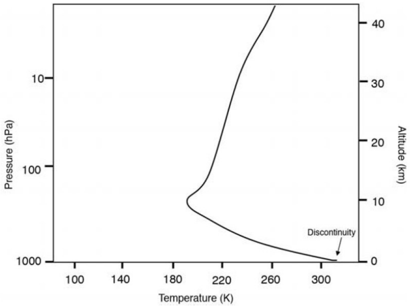


Figure: Radiative Equilibrium Profile

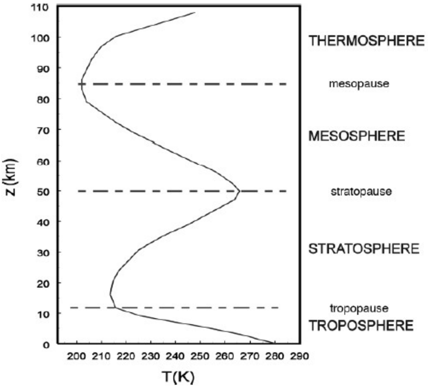
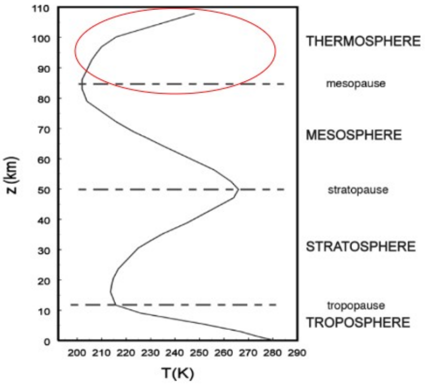


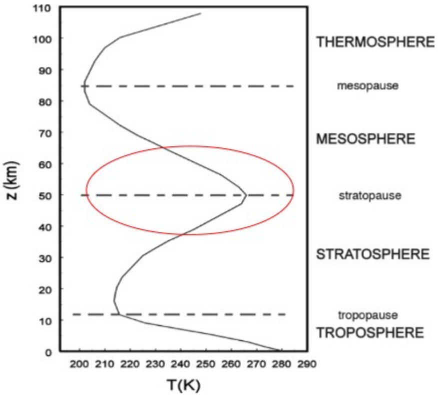
Figure: Typical Temperature Profile

Thermosphere



- The first hotspot, high and variable temperatures.
- Absorption of short wavelength UV ($\lambda < 0.1\mu m$) by O_2 and CO_2.
- Dissociation of the molecules is the reason for the high temperatures.
- Assumptions of thermodynamic equilibrium and blackbody radiation do not hold.
- Due to ionization processes, the ionosphere is formed in this region.

Mesosphere



- The layer below the mesopause at about 80-90 km, temperature increases through the mesosphere
- Next point of maxima/ second hotspot: stratopause
- Absorption of medium length UV ($0.1\mu m \leq \lambda \leq 0.35\mu m$) by O_3

Concentration of Ozone

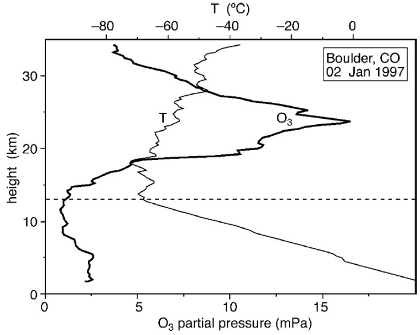


Figure: Typical Ozone Profile, dark line represents partial pressure of O_3 and light line represents temperature in Celsius

- Concentration of ozone varies in this region
- Photodissociation of ozygen:

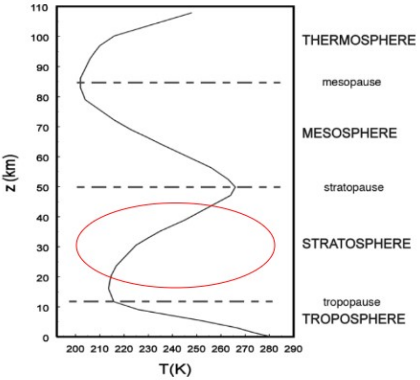
$$O_2 + h\nu \rightarrow O + O$$

$$O + O_2 + M \rightarrow O_3 + M$$

M is a third body required to carry excess energy.

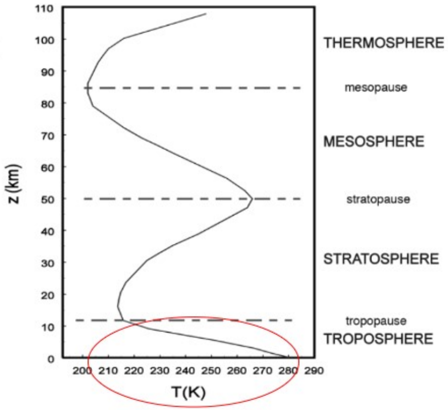
- Peak concentration is at 20 - 30 km altitude (stratosphere).
- The consequence of the peak being at lower altitudes makes all the difference to life on Earth.

Stratosphere



- "stratus" - layered, highly stratified region
- Poorly mixed and long residence times for particles ejected into it.
- Close to radiative equilibrium.
- The ozone and its radiative properties are the reason for the formation of the stratosphere.
- Important layer due to the presence of ozone as the primary UV absorber.

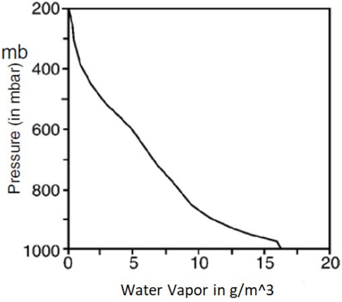
Troposphere



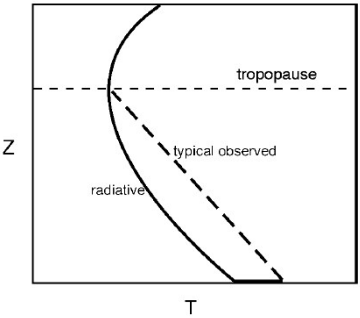
- Lies below the tropopause, with temperature increasing strongly moving towards the surface.
- Warm because of the absorption of radiation from the Sun and the surface by CO_2.
- Contains about 85% of the atmospheric mass and almost all water vapour.
- "Weather" is located here.

Radiative Equilibrium Profile

- Distribution of water vapour and the Clausius-Clayperon relation.
- The radiative equilibrium profile seen before is calculated for the troposphere from the vertical distribution of O_3, H_2O and CO_2.



(a) Vertical distribution of water vapour against pressure



(b) Radiative equilibrium profile in the troposphere

Quantum Mechanics of Greenhouse Gases

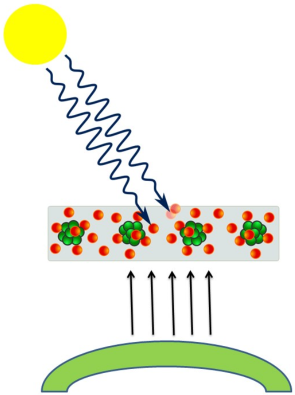


Figure: Picture taken from Wikipedia, edited.

- Consider a large number of quantum systems (molecules) in a radiation field.
- The transition between two states $|i\rangle \longleftrightarrow |k\rangle$ happens with energy $E_i = E_k + h\nu$.

Transition Matrix Elements

- The Einstein coefficients give the probability per unit time for absorption and spontaneous emission of radiation by the molecules.

$$\frac{dP_{ki}^{abs.}}{dt} = B_{ki}\ \omega(\nu)$$

$$\frac{dP_{ki}^{sp.em.}}{dt} = A_{ik}$$

- The Einstein Coefficients depend dominantly on the dipole transition matrix elements

$$\vec{M_{ik}} = \int \psi_i \vec{d} \psi_k \ d\tau$$

-

$$A_{ik} = \frac{2}{3}\frac{\omega_{ik}^3}{\epsilon_0 h c^3}|M_{ik}|^2$$

$$B_{ki} = \frac{2}{3}\frac{\pi^2}{\epsilon_0 h^2}|M_{ik}|^2$$

Diatomic Molecules

- The Hamiltonian of the system is

$$H=-\frac{\hbar^2}{2}\sum_{k=1}^{2}\frac{1}{M_k}\nabla_k^2-\frac{\hbar^2}{2m_e}\sum_{i=n}^{N}\nabla_i^2+\frac{e^2}{4\pi\epsilon_0}\left[\frac{Z_1Z_2}{R}+\sum_{i,j}\frac{1}{r_{i,j}}-\sum_i\left(\frac{1}{r_{i1}}+\frac{1}{r_{i2}}\right)\right]$$

$$\sim E_{kin}^{nucl}+E_{kin}^{el}+E_{pot}^{Coul}$$

- Applying the Born-Oppenheimer approximation
- Separation ansatz:

$$\psi(\vec{r_i},\vec{R_k})=\chi(\vec{R_k})\phi(\vec{r_i},R)$$

- $E_{pot}=\langle E_{kin}^{el}\rangle+E_{pot}^{Coul}$
- Rotational energy levels:

$$E_{rot}=\frac{J(J+1)\hbar^2}{2MR_e^2}$$

- Vibrational energy levels

$$E_{vib}=\hbar\omega_0\left(n+\frac{1}{2}\right)$$

Energy Levels of Diatomic molecules

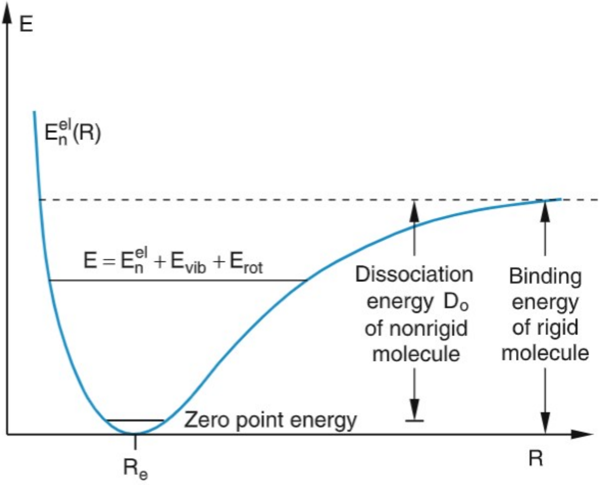


Figure: Potential Curve (Demtröder)

Spectra of Diatomic Molecules

- Dipole Matrix element

$$\vec{M_{ik}} = \int \chi_i^* \left[\int \phi_i \vec{d_{el}} \phi_k d\tau_{el} \right] \chi_k d\tau_N + \int \chi_i^* \vec{d_N} \left[\int \phi_i^* \phi_k d\tau_{el} \right] \chi_k d\tau_N$$

- Electronic transitions: $\phi_i \neq \phi_k, \chi_i = \chi_k$ corresponds to wavelengths $\simeq 200 \ - \ 700 \ nm$, which is visible/UV light.
- Vibrational-rotational transitions: $\phi_i = \phi_k, \chi_i \neq \chi_k$

$$\vec{M_{ik}} = \int \chi_i^* \vec{d_N} \chi_k d\tau_N$$

$$(n_i, J_i) \leftrightarrow (n_k, J_k) \begin{cases} \text{for} n_i \neq n_k : \text{Infrared region}, \ \lambda \sim 2\mu m - 20\mu m \\ \text{for} n_i = n_k : \text{Microwave region}, \ \lambda \sim 10^{-1} - 10^{-5} m \end{cases}$$

- For homonuclear molecules: $\vec{d_N} = 0$ so $\vec{M_{ik}} = 0$. These molecules absorb/emit (almost) no IR radiation. eg: O_2 and N_2

Energy Hierarchy for transitions

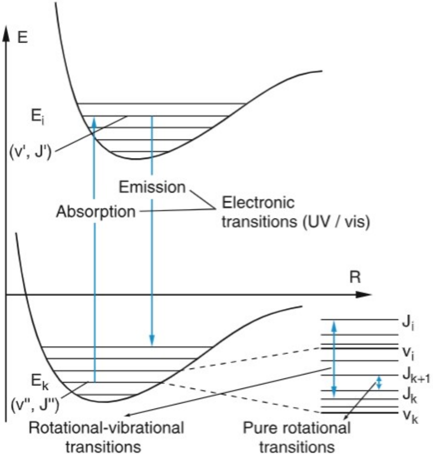


Figure: Structure of Molecular Transitions (Demtröder)

Polyatomic Molecules

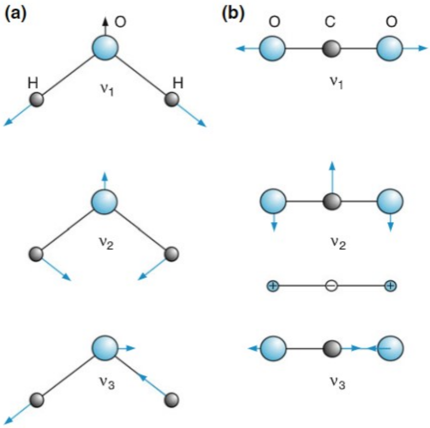
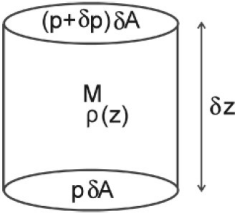


Figure: Normal vibrations for triatomic molecules H_2O and CO_2 (Demtröder)

- Electronic transitions: visible/UV range
- Pure rotational transitions: microwave range
- Vibrations are decomposed into normal vibrations
- Normal vibrations that change the dipole moment are infrared-active

Hydrostatic Balance



Consider a fluid column, with height δz and area of cross-section δA. The pressure $p(z)$ and density $\rho(z)$ are functions of height.

- The pressure at the top is

$$p_{top} = p(z + \delta z) = p(z) + \delta p$$

- As $\delta z \to 0$,

$$\delta p = \frac{\partial p}{\partial z} \delta z$$

- The mass of the cylinder is given by

$$M = \rho \times \delta A \times \delta z$$

Hydrostatic Balance

Assumption: The fluid column is subject to a net force of zero.
Sign Convention: Upwards is positive
Forces acting on the fluid column:

- Gravitational Force:
  $F_g = -g \times M = -g \times \rho \times \delta A \times \delta z$
- Force from pressure at the top
  $F_{top} = -P_{top} \times \delta A = -(p + \delta p) \times \delta A$
- Force from pressure at the bottom
  $F_{bottom} = p \times \delta A$

Adding up the forces: $F_g + F_{top} + F_{bottom} = 0$

Equation of Hydrostatic Balance

$$\frac{\partial p}{\partial z} + g\rho = 0$$

Estimating the Mass of the Atmosphere

As $z \to \infty$, $p \to 0$.

Integrating the equation of hydrostatic balance:

$$p(z) = g \int_{z}^{\infty} \rho dz$$

From the surface, with Earth's surface pressure (p_s) this becomes:

$$p_s = g \int_{surface}^{\infty} \rho dz$$

If m is the mass per unit area of a vertical column of unit cross section:

$$m = \frac{p_s}{g}$$

The mass of the atmosphere (M_a) is then:

$$M_a = \frac{p_s}{g} \times surface\ area\ of\ Earth$$

Estimating the Mass of the Atmosphere

Plugging in values:
Surface pressure

$$p_s \approx 1 \ bar = 10^5 \ Pa$$

Gravitational acceleration

$$g = 9.81 \ m/s^2$$

Radius of Earth

$$r = 6.37 \times 10^6 m$$

$$M_a = \frac{p_s}{g} \times 4\pi \ r^2$$

Mass of the atmosphere can be calculated as:

$$M_a = 5 \times 10^{18} \ kg$$

Estimating the Mass of the Atmosphere

How good are the assumptions made?

Atmospheric mass	M_a	5.26×10^{18} kg
Global mean surface pressure	p_s	1.013×10^{5} Pa
Global mean surface temperature	T_s	288 K
Global mean surface density	ρ_s	$1.235\ \mathrm{kg\,m^{-3}}$

Figure: Table from Chapter 1 of Marshall and Plumb

Vertical Structure of Pressure and Density

The equation of the state of air is

$$p = \rho \times R \times T$$

Applying this to the equation of hydrostatic balance

$$\frac{\partial p}{\partial z} = -\frac{g}{R}\frac{p}{T}$$

Is this substitution useful?

Two main cases to be considered:

- T is a constant
- T varies with height

Isothermal Atmosphere

Assumption: $T = T_0$ is a constant.
Hydrostatic balance equation becomes:

$$\frac{\partial p}{\partial z} = -\frac{g\ p}{R\ T_0} = -\frac{p}{H}$$

Define the quantity H, which is the scale height

$$H := \frac{R\ T_0}{g}$$

Solving the equation for p, taking the initial condition as $p = p_s$ for $z = 0$:

$$p(z) = p_s exp\left(-\frac{z}{H}\right)$$

$$ln(p(z)) = ln(p_s)\left(\frac{-z}{H}\right)$$

$$z = H\ ln\left(\frac{p_s}{p}\right)$$

Isothermal Atmosphere

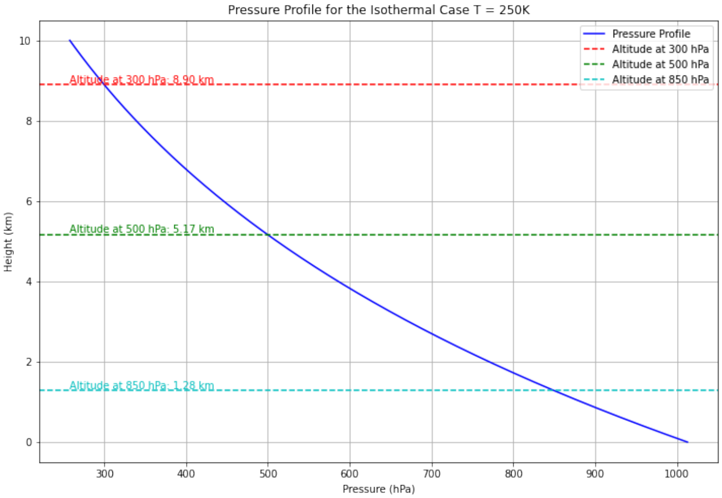


Figure: Pressure profile of the troposphere as predicted for isothermal atmosphere

Non-isothermal Atmosphere

Assumption: T is not a constant

Scale height is then defined as

$$H(z) = \frac{R\ T(z)}{g}$$

Hydrostatic balance equation becomes

$$\frac{\partial p}{\partial z} = -\frac{p}{H(z)}$$

Solving this equation:

$$\frac{1}{p}\frac{\partial p}{\partial z} = \frac{\partial(ln(p))}{\partial z} = -\frac{1}{H(z)}$$

$$ln(p) = \int_0^z \frac{dz'}{H(z')} + constant$$

$$p(z) = p_s\ exp\left(-\int_0^z \frac{dz'}{H(z')}\right)$$

Case in Reality

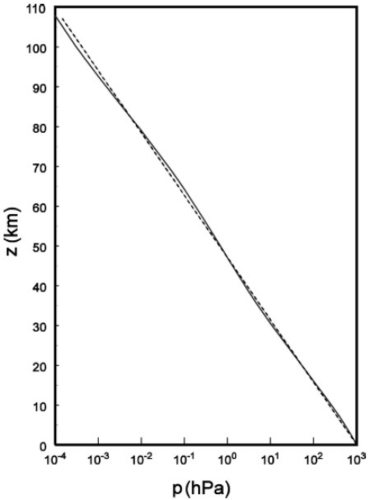


Figure: Observed pressure profile (solid line) plotted against the theoretical isothermal case (dashed line) from Marshall and Plumb.

Density

For the isothermal case, density can be obtained from the equation for pressure:

$$\rho(z) = \frac{p_s}{R_0} exp\left(-\frac{z}{H}\right)$$

For the non-isothermal case:

$$\rho(z) = \frac{p_s}{R\ T(z)} exp\left(-\int_0^z \frac{dz'}{H(z')}\right)$$

Consequence of this: explains why the mass of the atmosphere is concentrated in the first few regions.

Isothermal Density Profile

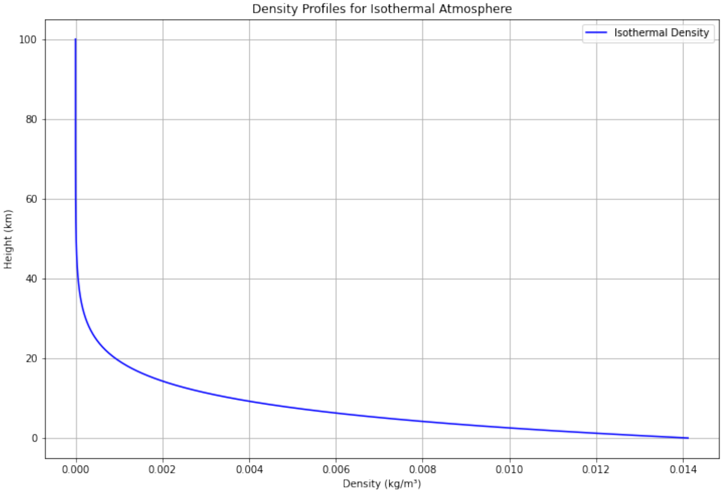


Figure: Density profile for an isothermal atmosphere

Effects of Climate Change

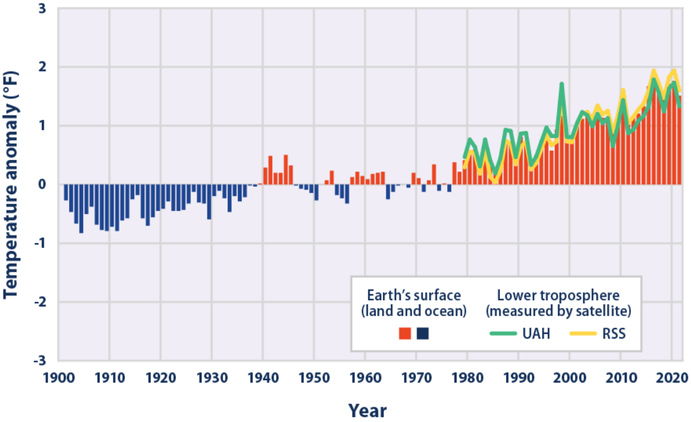


Figure: Worldwide change in annual average temperatures from 1901-2021. Data from EPA.gov

Effects of Climate Change

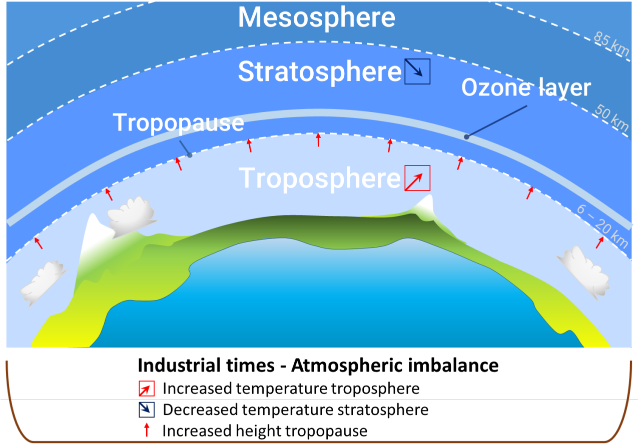


Figure: Representation of an increase in temperature of troposphere, cooling of stratosphere and increased height of troposphere based on a study by IPCC (2021) (Picture from EUMETSAT)

Effects of Climate Change

HOME > SCIENCE ADVANCES > VOL. 7, NO. 45 > CONTINUOUS RISE OF THE TROPOPAUSE IN THE NORTHERN HEMISPHERE OVER 1980–2020

RESEARCH ARTICLE | CLIMATOLOGY

Continuous rise of the tropopause in the Northern Hemisphere over 1980–2020

LINGYUN MENG, JANE LIU, DAVID W. TARASICK, WILLIAM J. RANDEL, ANDREA K. STEINER, HALLGEIR WILHELMSEN, LEI WANG, AND LEOPOLD HAIMBERGER Authors Info & Affiliations

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Figure: Paper by Meng et al. from the University of Toronto published November 2021 on the increase in height of the tropopause.

Effects of Climate Change

RESEARCH ARTICLE | EARTH, ATMOSPHERIC, AND PLANETARY SCIENCES |

Exceptional stratospheric contribution to human fingerprints on atmospheric temperature

Benjamin D. Santer, Stephen Po-Chedley, Lilong Zhao, +5, and Karl E. Taylor Authors Info & Affiliations

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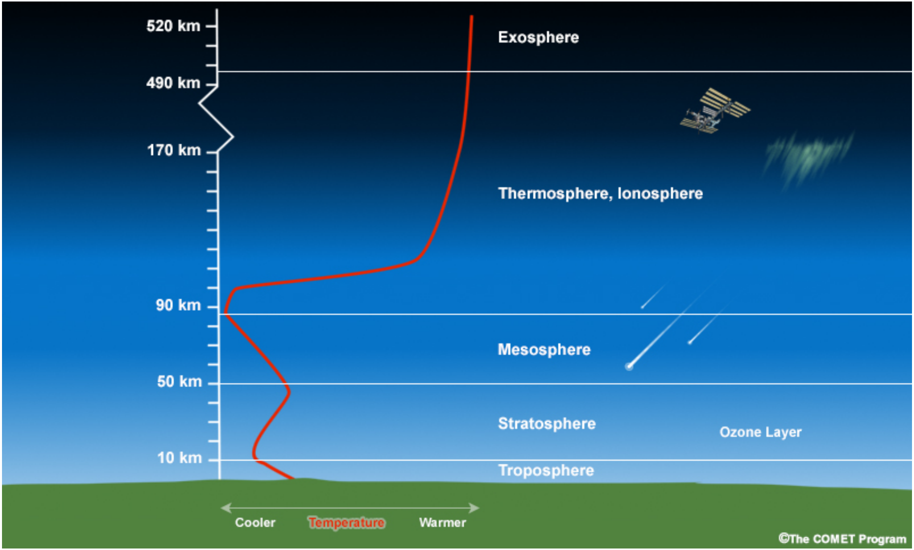
May 8, 2023 | 120 (20) e2300758120 | https://doi.org/10.1073/pnas.2300758120

Figure: Paper by Santer et al. from UCLA published May 2023 on the anthropogenic cooling of the stratosphere.

The End


520 km
490 km
170 km
90 km
50 km
10 km
Exosphere
Thermosphere, Ionosphere
Mesosphere
Stratosphere
Ozone Layer
Troposphere
Cooler
Temperature
Warmer
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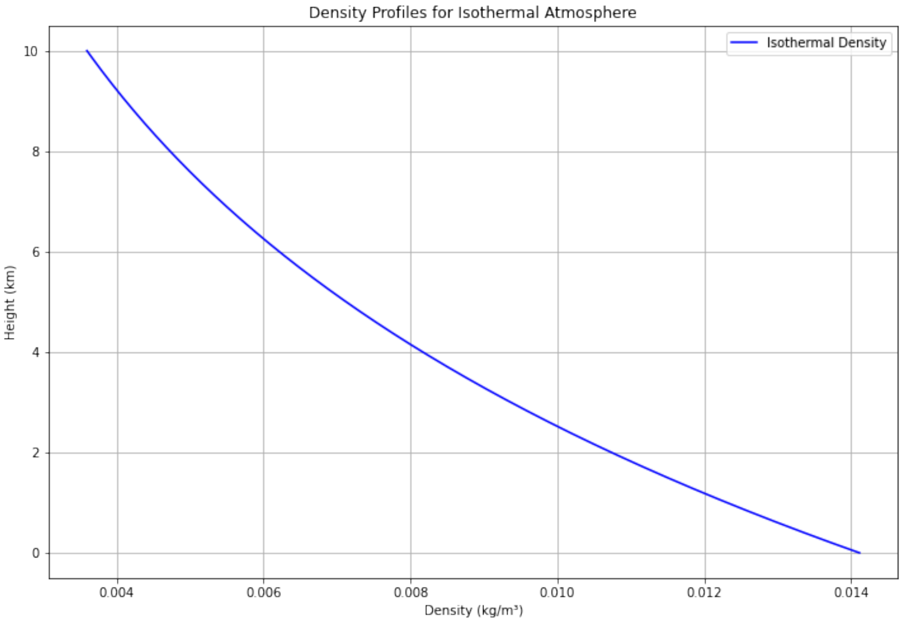
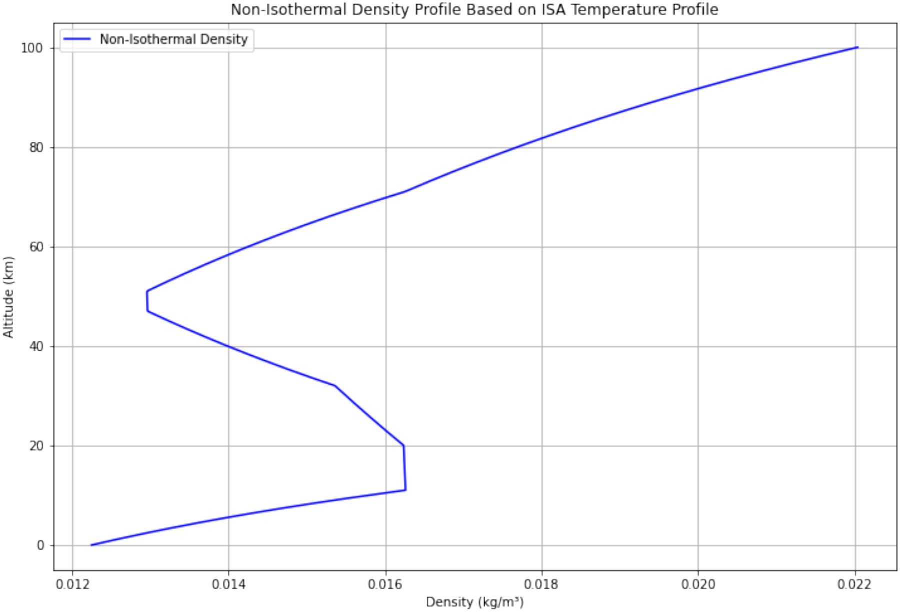


Density Profiles for Isothermal Atmosphere
Isothermal Density
Height (km)
Density (kg/m³)
0
2
4
6
8
10
0.004
0.006
0.008
0.010
0.012
0.014


Non-Isothermal Density Profile Based on ISA Temperature Profile
Non-Isothermal Density
Altitude (km)
0
20
40
60
80
100
0.012
0.014
0.016
0.018
0.020
0.022
Density (kg/m³)

Effects of Climate Change

"Early climate modelers predicted back in the 1960s that this combination of tropospheric warming and strong cooling higher up was the likely effect of increasing CO_2 *in the air. But its recent detailed confirmation by satellite measurements greatly enhances our confidence in the influence of* CO_2 *on atmospheric temperatures, says Santer, who has been modeling climate change for 30 years.*
This month, he used new data on cooling in the middle and upper stratosphere to recalculate the strength of the statistical "signal" of the human fingerprint in climate change. He found that it was greatly strengthened, in particular because of the additional benefit provided by the lower level of background "noise" in the upper atmosphere from natural temperature variability. Santer found that the signal-to noise ratio for human influence grew fivefold, providing "incontrovertible evidence of human effects of the thermal structure of the Earth's atmosphere." We are "fundamentally changing" that thermal structure, he says. "These results make me very worried.""