GF 3022

- Ecuación de continuidad en la vida real
  - Tratamiento del término de turbulencia
- Composición y estructura atmosféricas
- Emisiones

Conservación de masa para cada traza

+CB **+CI**

Variación por advección
por el flujo promedio

$$\frac{\partial c}{\partial t} = -\vec{v}.\nabla c - c\nabla.\vec{v} - \nabla.(<c'\vec{v}'>) + Q - S$$

Variación por
flujos turbulentos

Variación por convergencia
o divergencia del aire

Variación Local
de la concentración

Fuentes y Sumideros

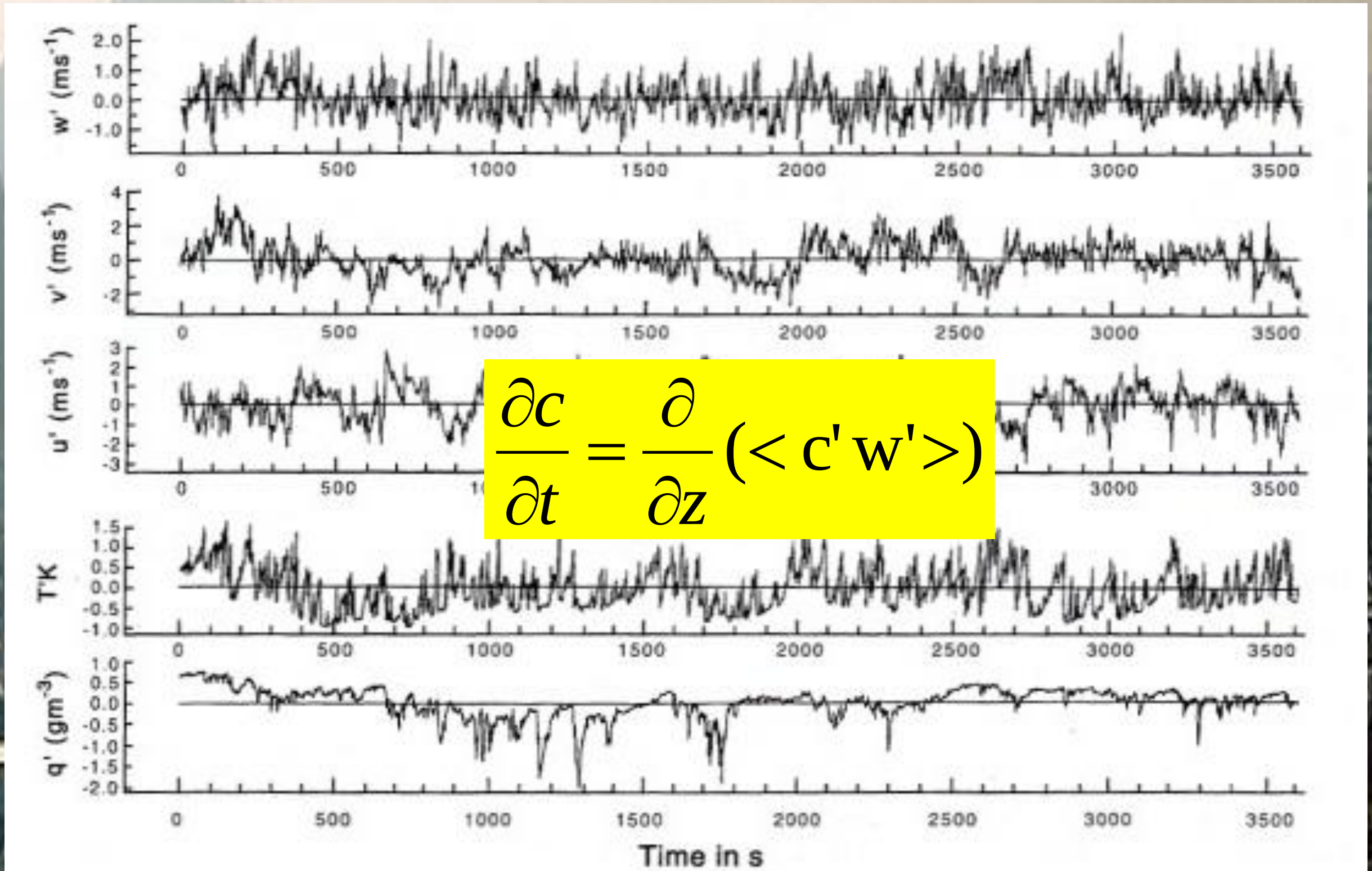
À la Euler....modelos Eulerianos

$$\frac{\partial c}{\partial t} = -\vec{\mathrm{v}}.\nabla c - c\nabla.\vec{\mathrm{v}} - \nabla.(<\mathrm{c}'\vec{\mathrm{v}}'>) + Q - S$$

À la Lagrange...modelos Lagrangianos

$$\frac{dc}{dt} = -c\nabla.\vec{\mathrm{v}} - \nabla.(<\mathrm{c}'\vec{\mathrm{v}}'>) + Q - S$$

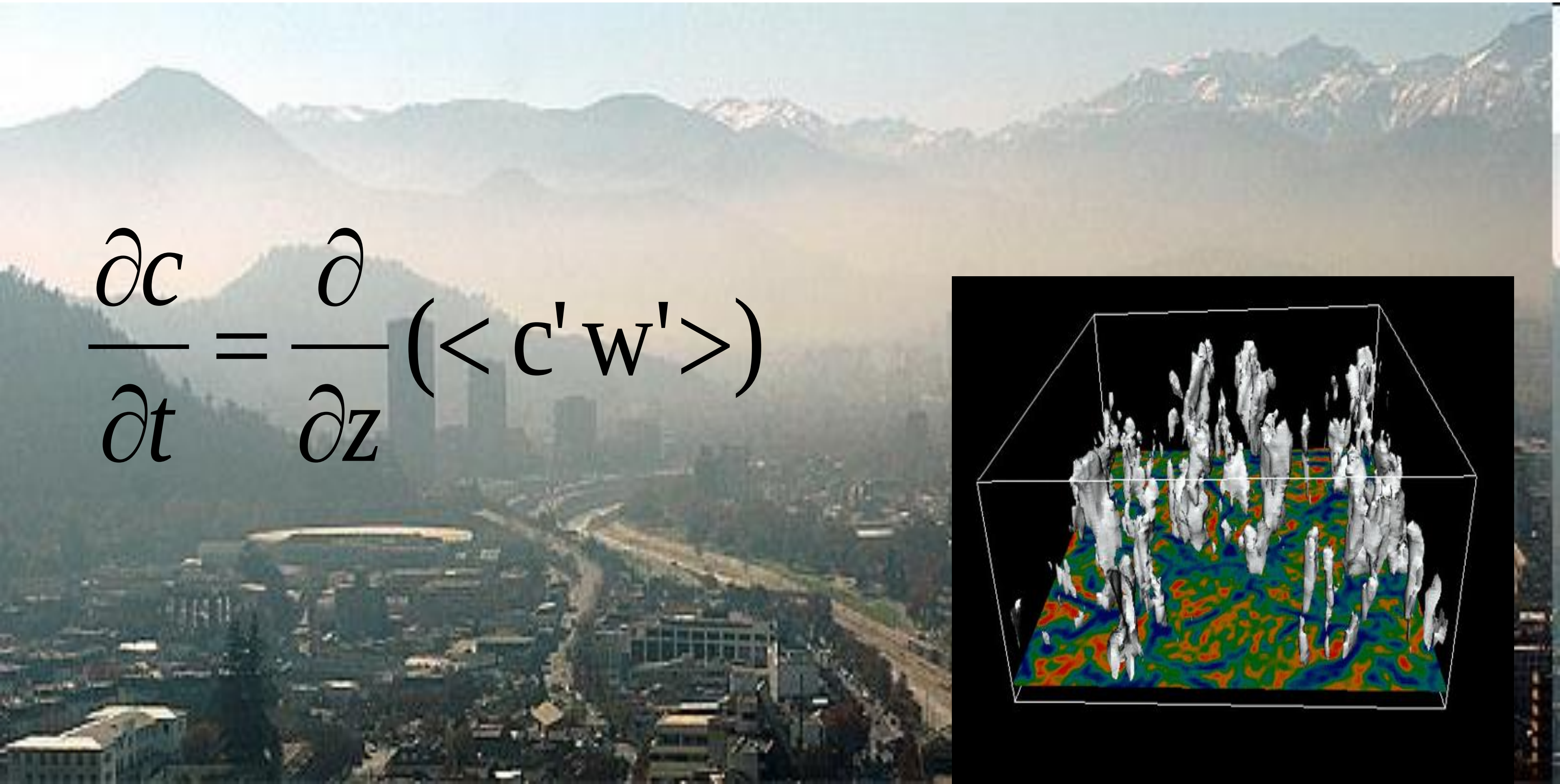
Turbulencia y fluctuaciones: hay transporte si hay cofluctuaciones y gradientes verticales



$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}(< c' w' >)$$

Mezcla turbulenta

•Prevalece en la vertical (0 ~1 km)



$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}(< c' w' >)$$

Tratamiento usual: parametrización à la Fick

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}(< c' w' >) \approx -\frac{\partial}{\partial z}\left(K_{zz}\frac{\partial c}{\partial z}\right)$$

- La mezcla ocurre contra gradiente (-)
- Existe un coeficiente análogo al coeficiente de difusión molecular
- K_{zz} se parametriza y depende de las condiciones de estabilidad y mezcla
- Kzz se estima a través mediciones de alta frecuencia

Atmos. Chem. Phys. Discuss., 4, 1371–1392, 2004
www.atmos-chem-phys.org/acpd/4/1371/
SRef-ID: 1680-7375/acpd/2004-4-1371

Atmospheric Chemistry and Physics Discussions

3-D chemistry-transport model Polair: numerical issues, validation and automatic-differentiation strategy

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Received: 3 October 2003 – Accepted: 3 March 2004 – Published: 8 March 2004

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2. Model overview

As an Eulerian three-dimensional chemistry-transport model, Polair handles basic physical processes by integrating in time the following equation:

$$\frac{\partial c_i}{\partial t} + \operatorname{div}(c_i \cdot V) = \operatorname{div}(\mathbf{K} \cdot \nabla c_i) + \chi_i(c) - D_i + E_i \qquad (1)$$

where i labels a chemical species, c is a vector of chemical concentrations, V is the wind vector, $\mathbf{K}$ is the diffusion matrix, χ_i combines production and loss terms of chemi-

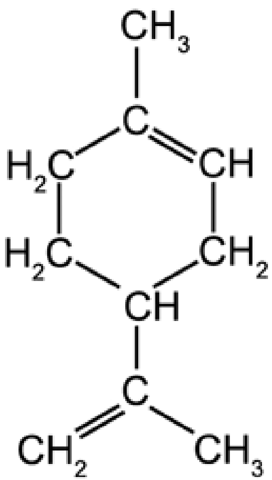
Ecuaciones de continuidad en la vida real…

$$\frac{\partial c_i}{\partial t} + \operatorname{div}(c_i \cdot V) = \operatorname{div}(\mathbf{K} \cdot \nabla c_i) + \chi_i(c) - D_i + E_i$$

vs.

$$\frac{\partial c}{\partial t} = -\vec{\mathrm{v}}.\nabla c - c\nabla.\vec{\mathrm{v}} - \nabla.(<\mathrm{c}'\vec{\mathrm{v}}'>) + Q - S$$

Ec. de continuidad de la vida real: el aroma de los bosques de cítricos (limonina)



$$L + OH \rightarrow \text{productos}, k1\,(R1)$$

$$k1 = 3.7\ \text{ppbv}^{-1}\ \text{s}^{-1}, \left[OH\right] \sim 1\,pptv$$

$$L + O_3 \rightarrow \text{productos}, k2\,(R2)$$

$$k2 = 1.6\,10^{-5}\ \text{ppbv}^{-1}\,\text{s}^{-1}, \left[O_3\right] \sim 60\,ppbv$$

¿Se puede despreciar el efecto de las reacciones con OH y O3 sobre la concentración (c) de la limonina a 70 m de altura sobre la capa de los árboles si uno compara con el efecto del transporte turbulento? (Supón pinos de 20 m de alto).

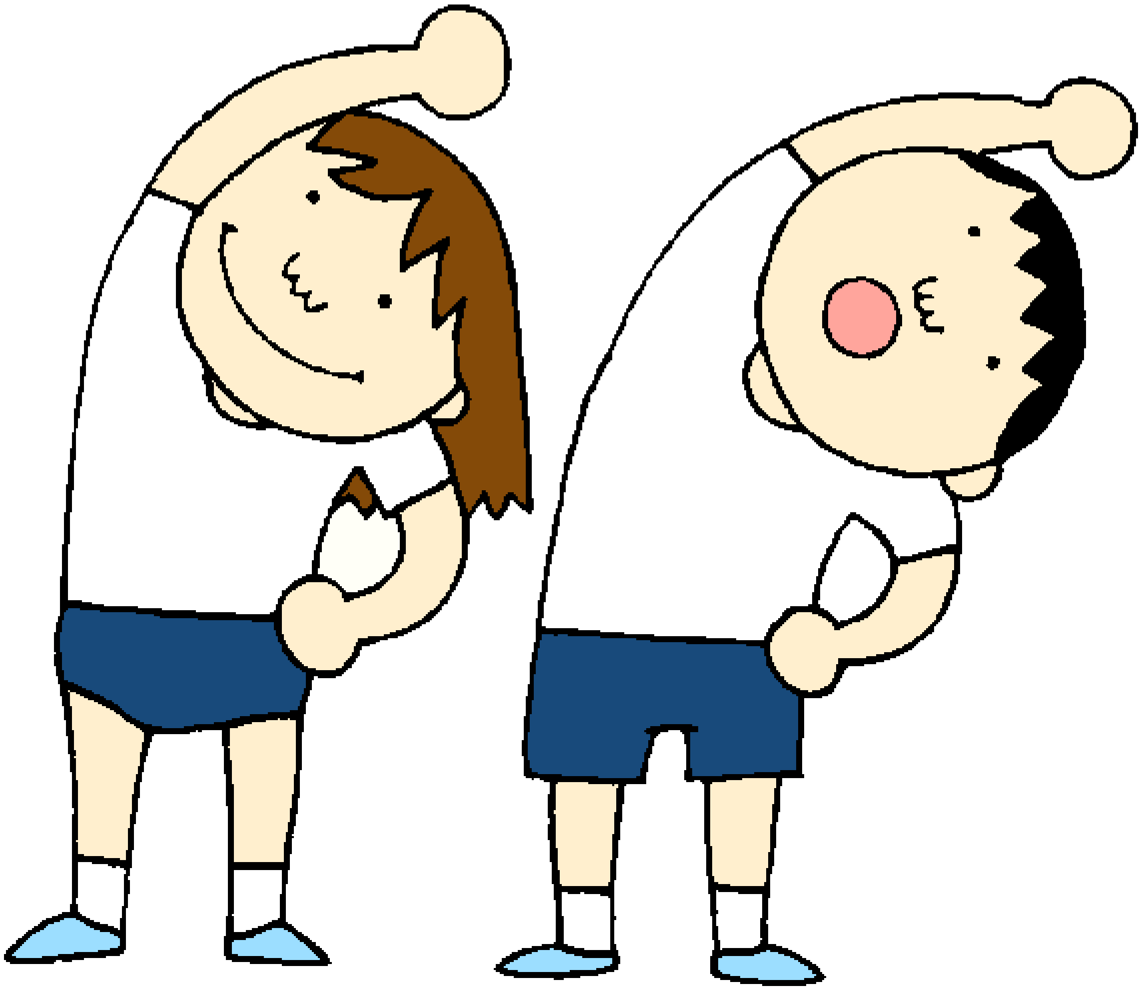
$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial z}\left(K_z \frac{\partial c}{\partial z}\right) - R1 - R2$$

$$K_z = 10\ m^2 s^{-1}$$

NB. Construye una escala de tiempo característica para la lezcla turbulenta

$$\tau = \frac{L^2}{K}$$

Pausa in situ…



Una envolvente, mayoritariamente gaseosa, muy tenue

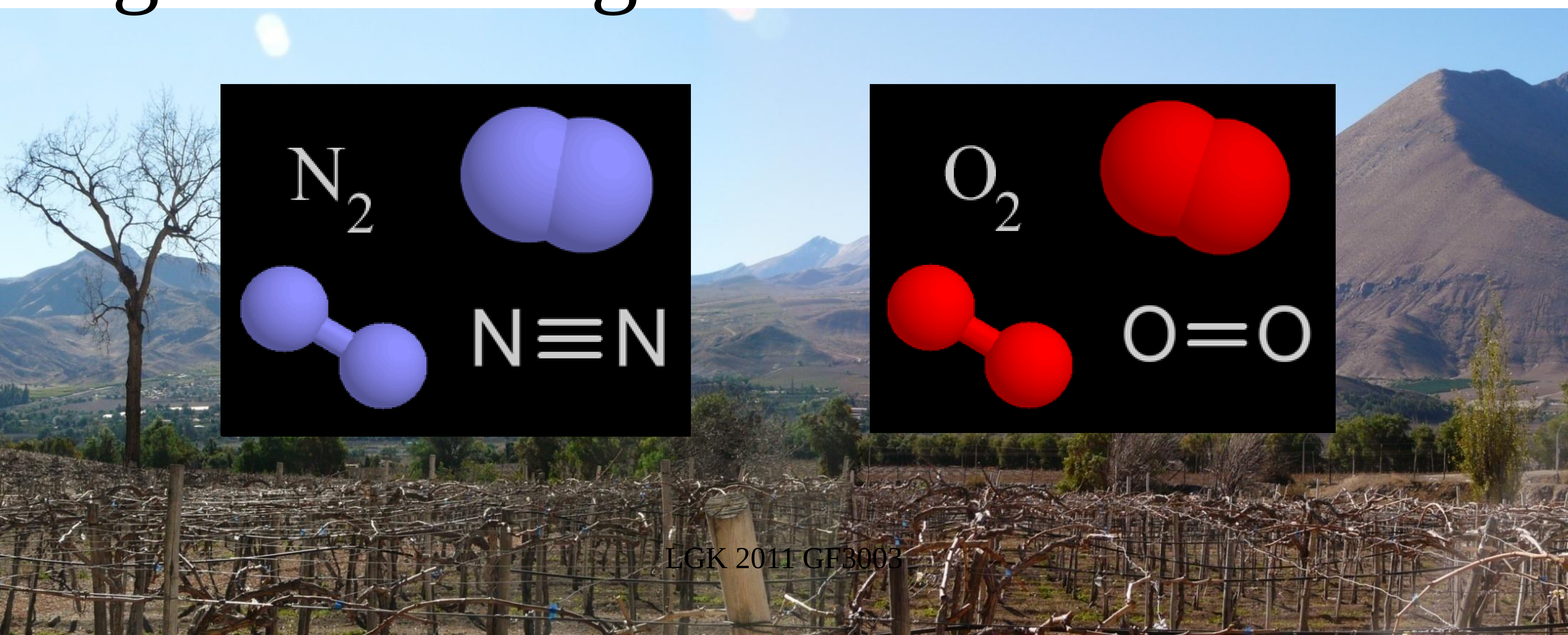
El espesor del fluido atmosférico ~100 km

Contando la capa ionizada ~600 km

Se compara con ~6300 km de radio terrestre

El compuesto más común (4/5~78%): nitrógeno molecular

Seguido de oxígeno molecular ~21%



Composición mayoritaria de la atmósfera

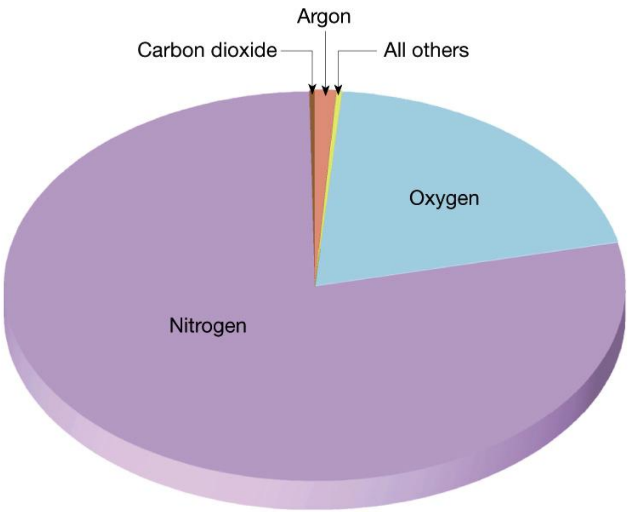
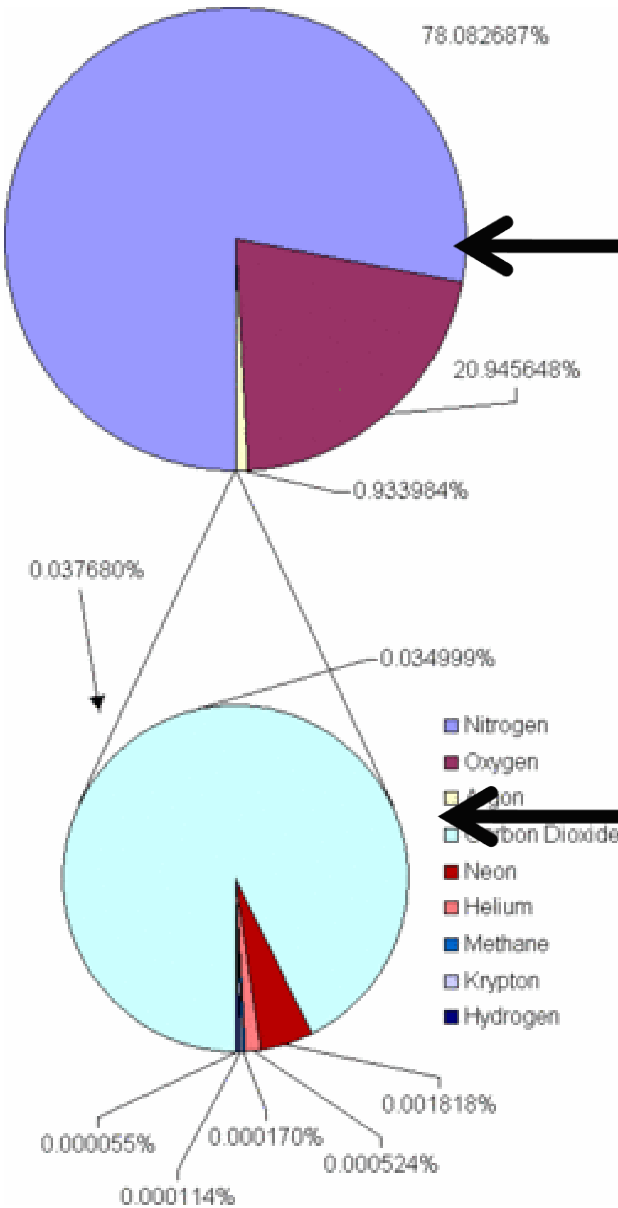


Table 1–2 Principal gases of dry air

Constituent	Percent by Volume	Concentration in Parts Per Million (PPM)
Nitrogen (N_2)	78.084	780,840.0
Oxygen (O_2)	20.946	209,460.0
Argon (Ar)	0.934	9,340.0
Carbon dioxide (CO_2)	0.036	360.0
Neon (Ne)	0.00182	18.2
Helium (He)	0.000524	5.24
Methane (CH_4)	0.00015	1.5
Krypton (Kr)	0.000114	1.14
Hydrogen (H_2)	0.00005	0.5

http://www.ux1.eiu.edu/~cfjps/1400/atmos_origin.html

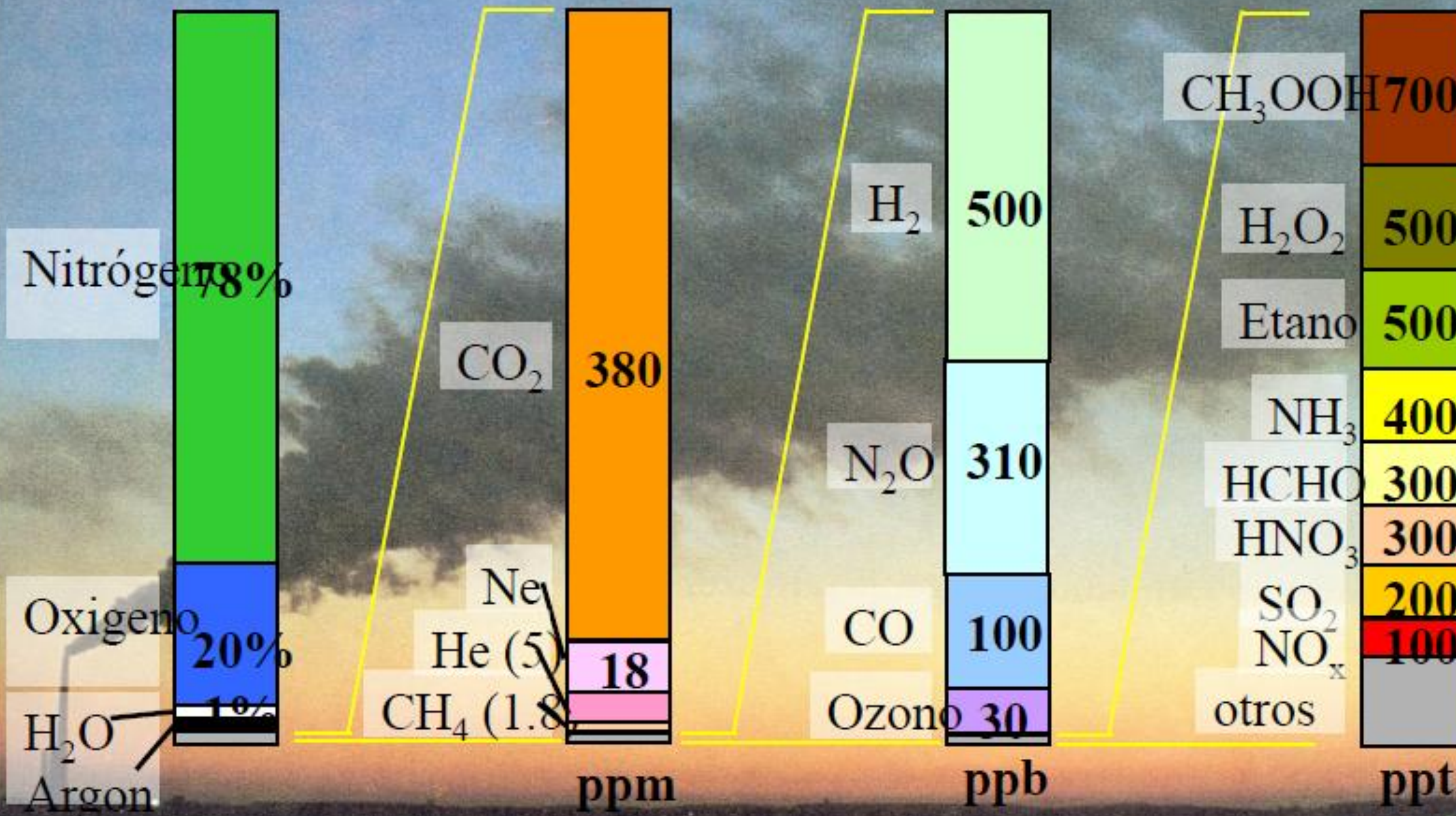
Otra manera de ver lo mismo



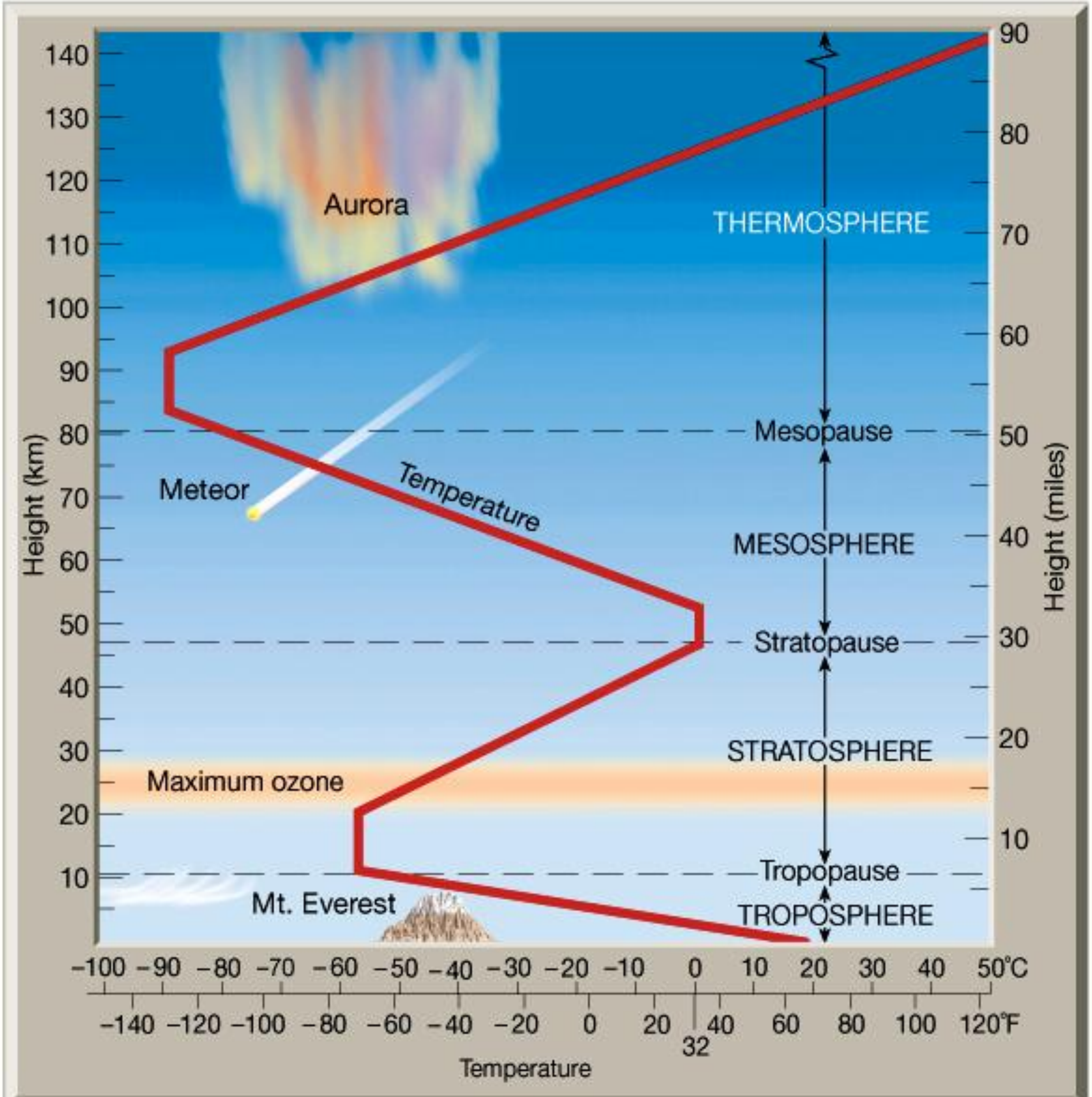
Definen las propiedades del fluido en términos de masa

Definen las propiedades del fluido en términos de química, biología, etc…y de energía

Composición de la Atmósfera



Gentileza de AMC

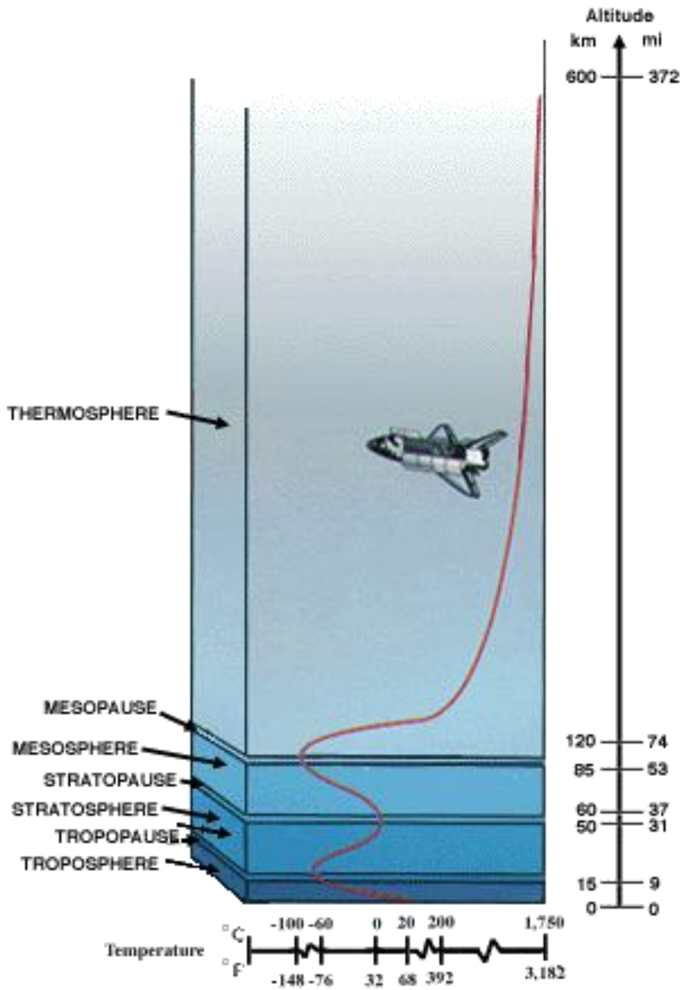


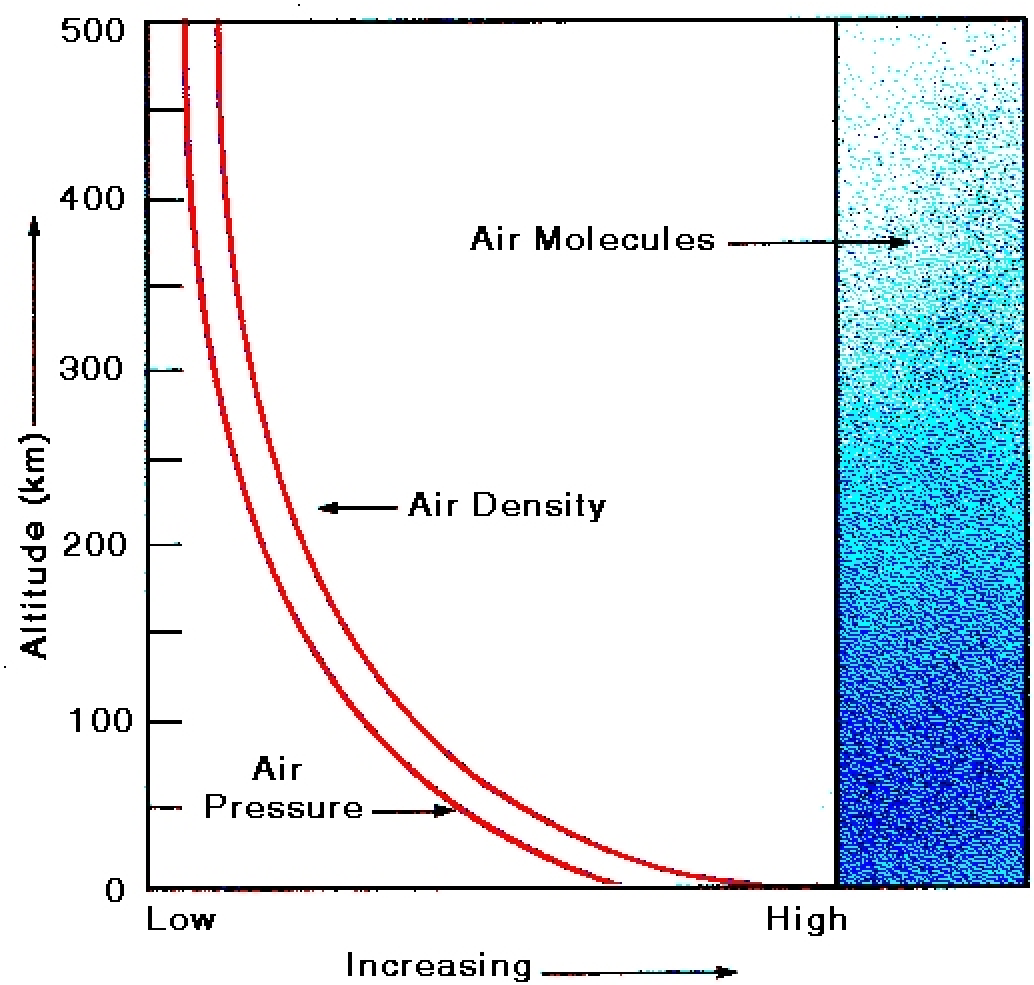
Aurora
THERMOSPHERE
Mesopause
Meteor
Temperature
MESOSPHERE
Stratopause
STRATOSPHERE
Maximum ozone
Tropopause
Mt. Everest
TROPOSPHERE
Height (km)
140
130
120
110
100
90
80
70
60
50
40
30
20
10
Height (miles)
90
80
70
60
50
40
30
20
10
−100 −90 −80 −70 −60 −50 −40 −30 −20 −10 0 10 20 30 40 50°C
−140 −120 −100 −80 −60 −40 −20 0 20 32 40 60 80 100 120°F
Temperature

En la atmósfera prevalecen los movimientos horizontales

Se comporta, grosso modo, como un gas ideal

Presión, temperatura y densidad definen una relación de estado termodinámico





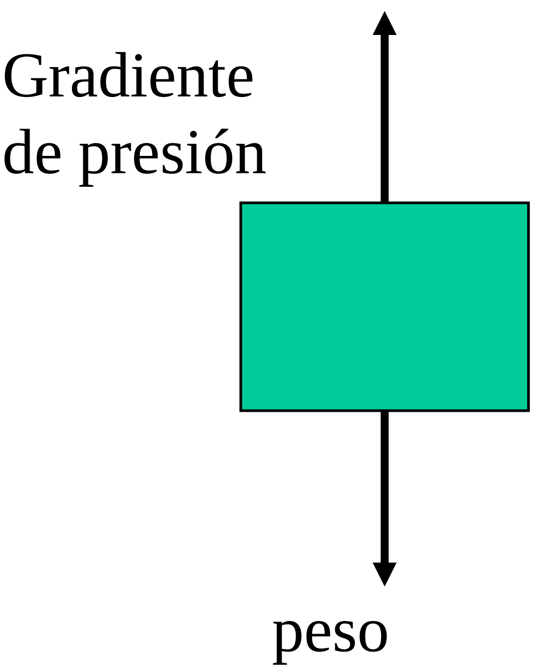
Atmósfera como gas ideal

$$pV = n R^* T = \frac{m}{M} R^* T$$

$$\boxed{\mathbf{p = \rho R T}}$$

$$R = \frac{R^*}{M} = 287 \left[\frac{J}{kg\,K} \right]; M \approx 29 \left[\frac{g}{mol} \right]$$

Balance hidrostático



“La atmósfera no se cae...”

La fuerza de gravedad (hacia abajo) es compensada por el gradiente vertical de presión (hacia arriba)

$$\boxed{\frac{\partial p}{\partial z} = -\rho g}$$

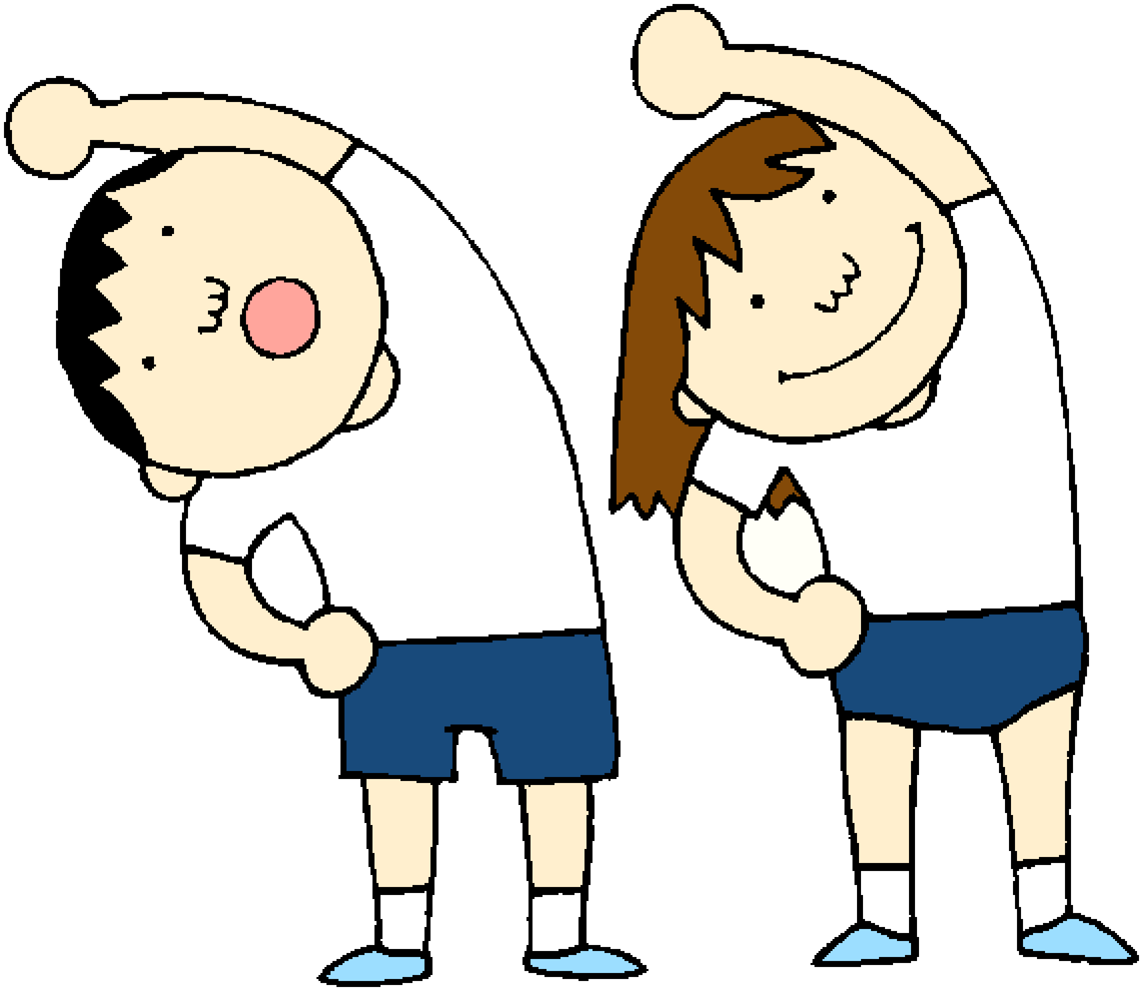
$$\boxed{p = \rho R T}$$

$$\boxed{\frac{\partial p}{\partial z} = -\rho g}$$

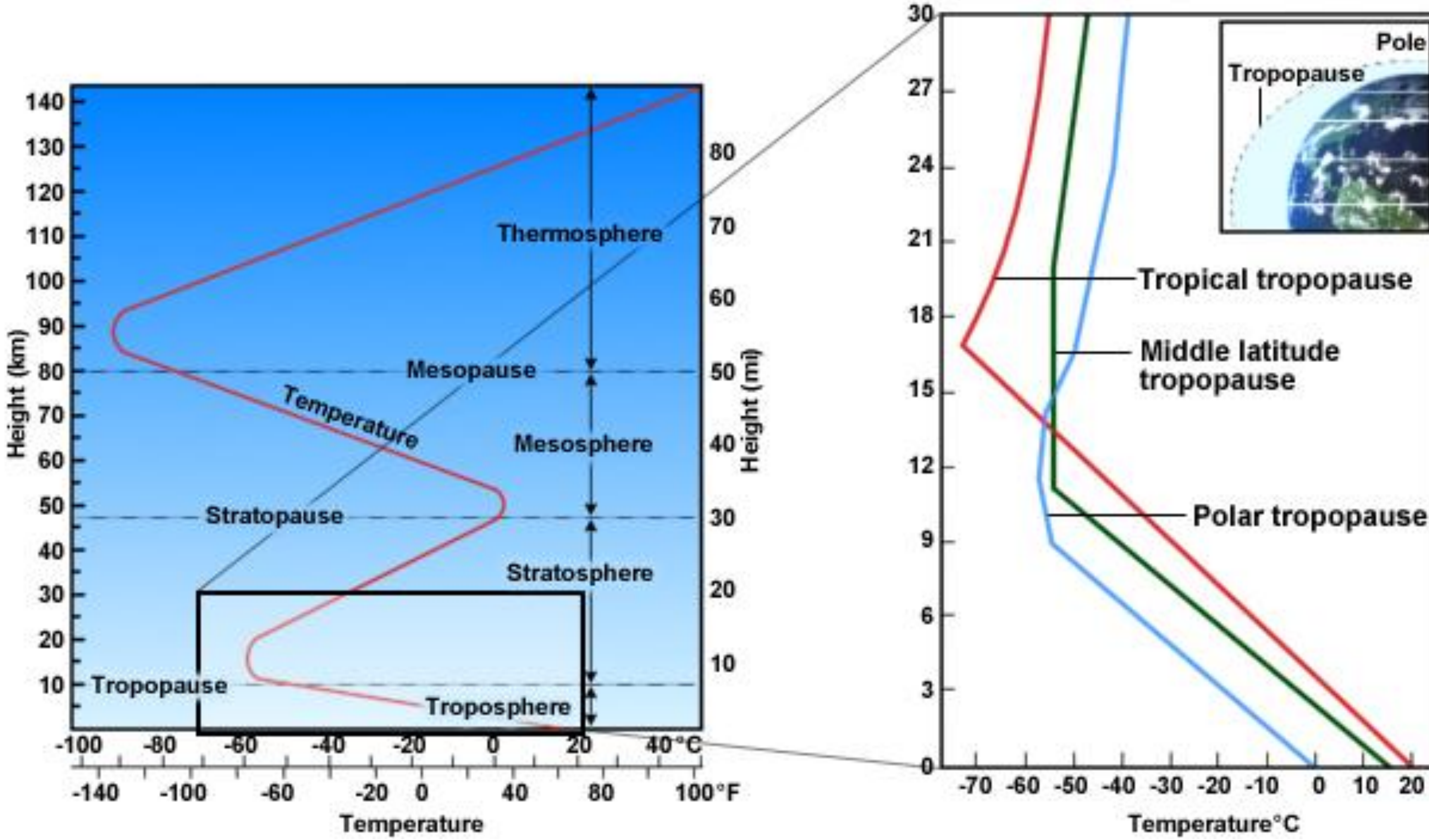
$$\boxed{\frac{\partial p}{p} = -\frac{g}{RT}\partial z = \frac{-\partial z}{H}}$$

Esto da una excelente aproximación de la variación vertical de la presión. Excepto en situaciones con movimientos verticales intensos, por ejemplo, tornados.

Pausa in situ…



¿Por qué desciende generalmente la temperatura en la tropósfera?

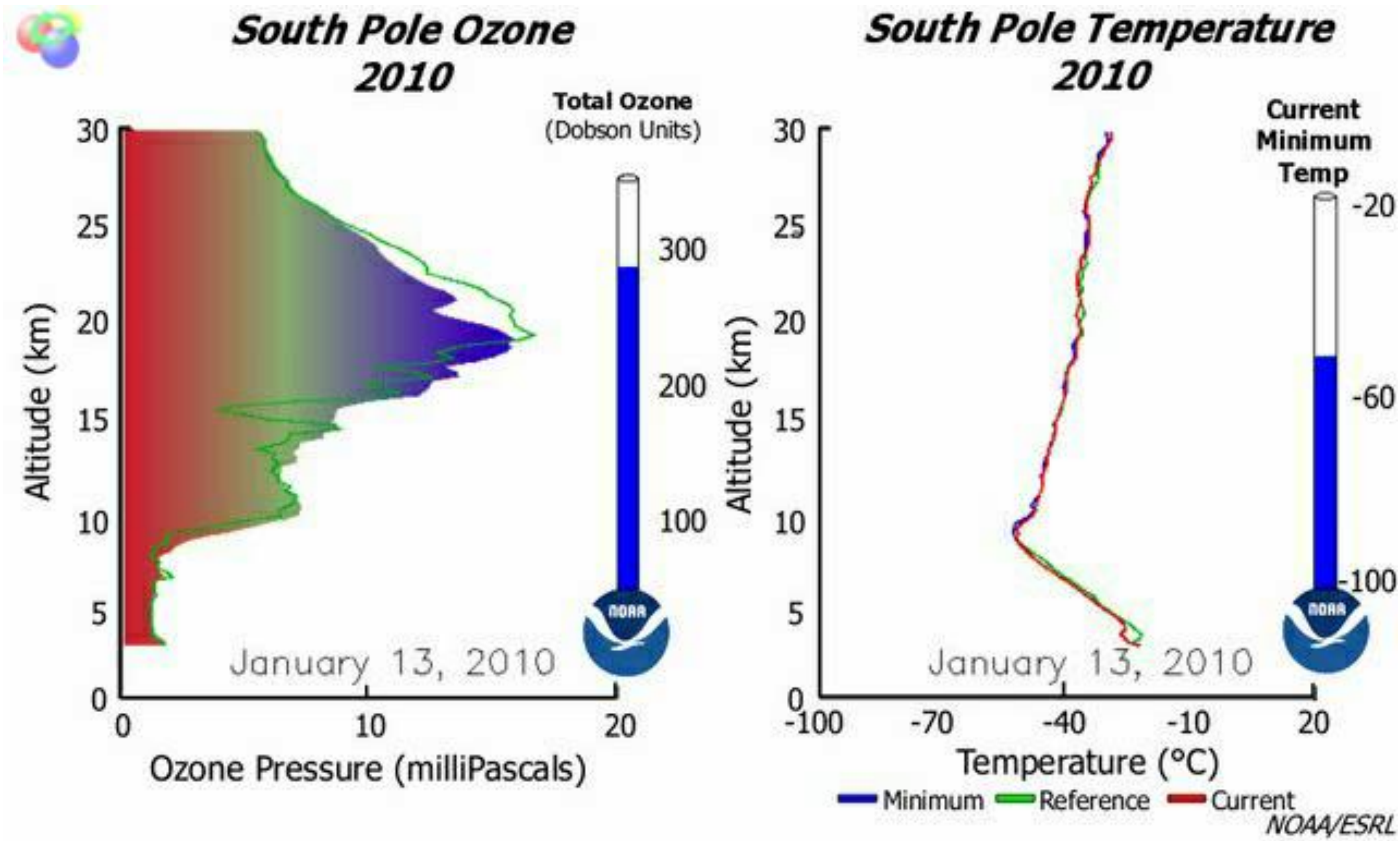


- La tropósfera, que contiene el 75% de la masa atmosférica, es calentada desde abajo (el sol calienta la superficie)
- La condición es termodinámicamente inestable (aire caliente por debajo de aire frío)

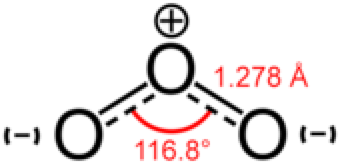
del griego τροπος *(tropos* = girar) y σφαιρα (sphaira = esfera).

http://www.meted.ucar.edu

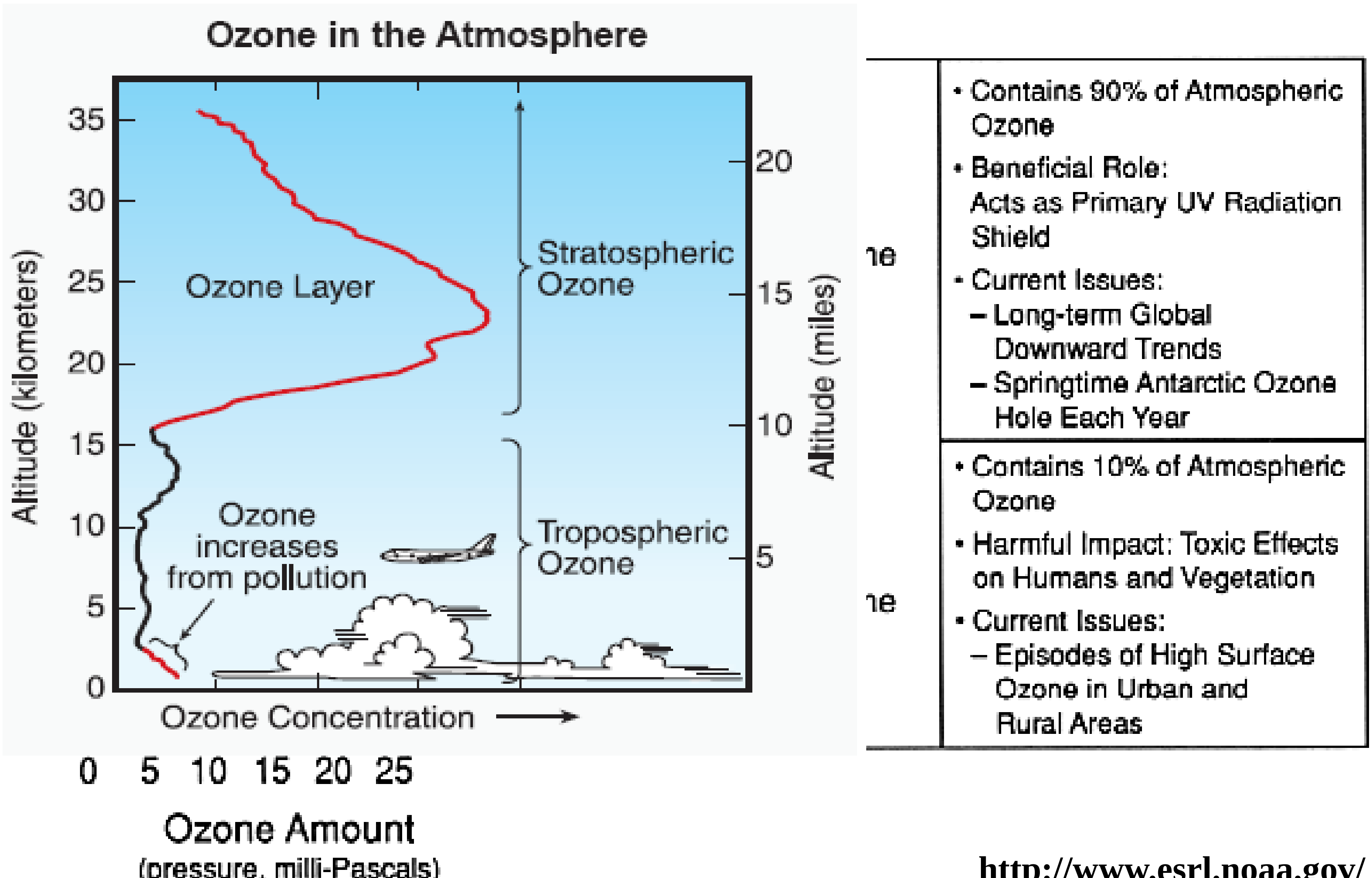
http://www.esrl.noaa.gov/gmd/dv/spo_oz/movies/index.html



La absorción de radiación UV por ozono en la estratósfera determina el máximo de temperatura

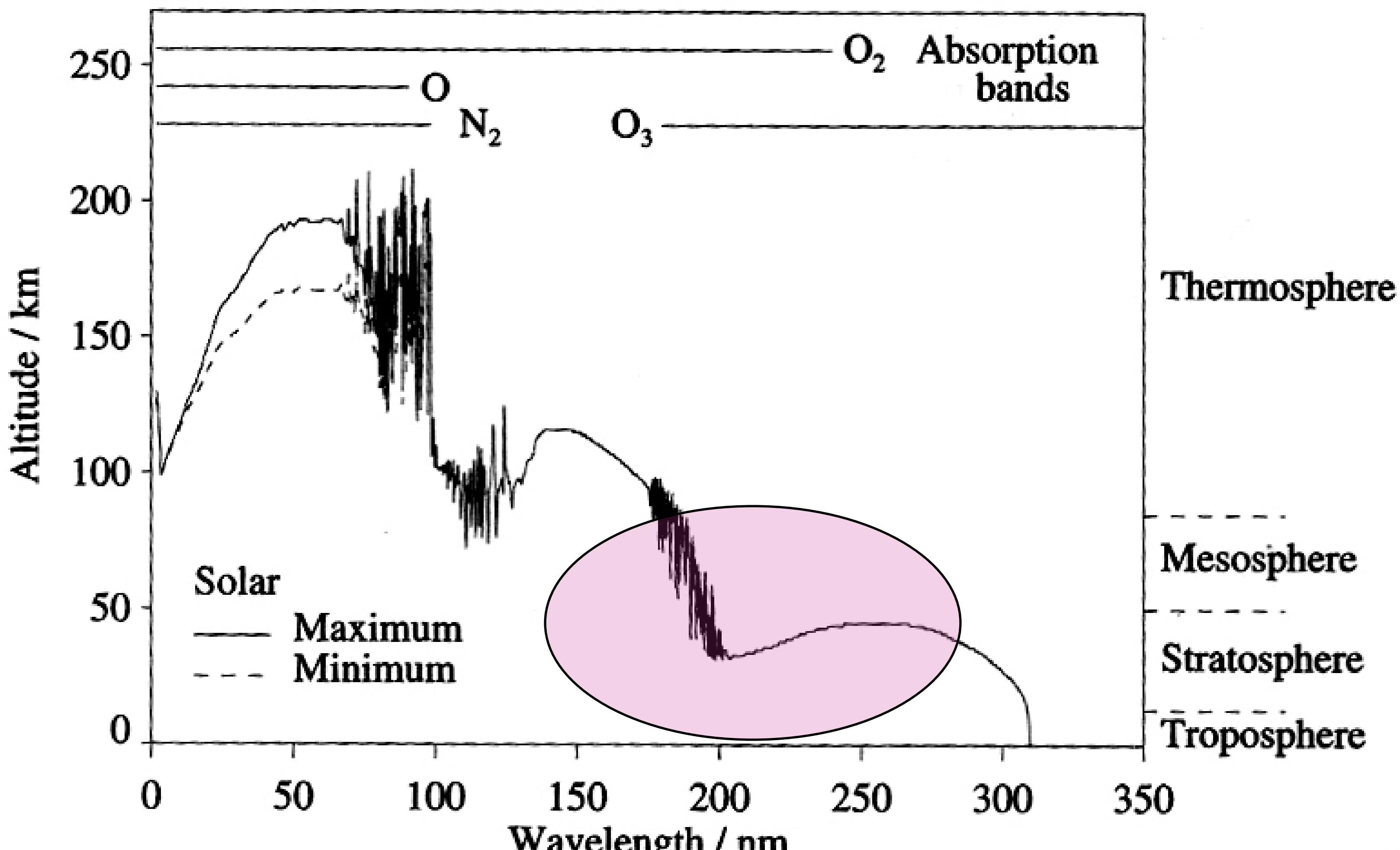


¿Dónde está el ozono?



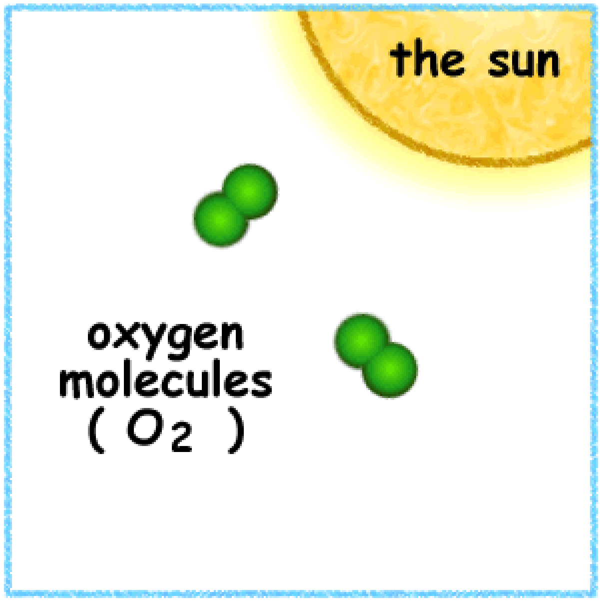
http://www.esrl.noaa.gov/

Absorción de radiación UV

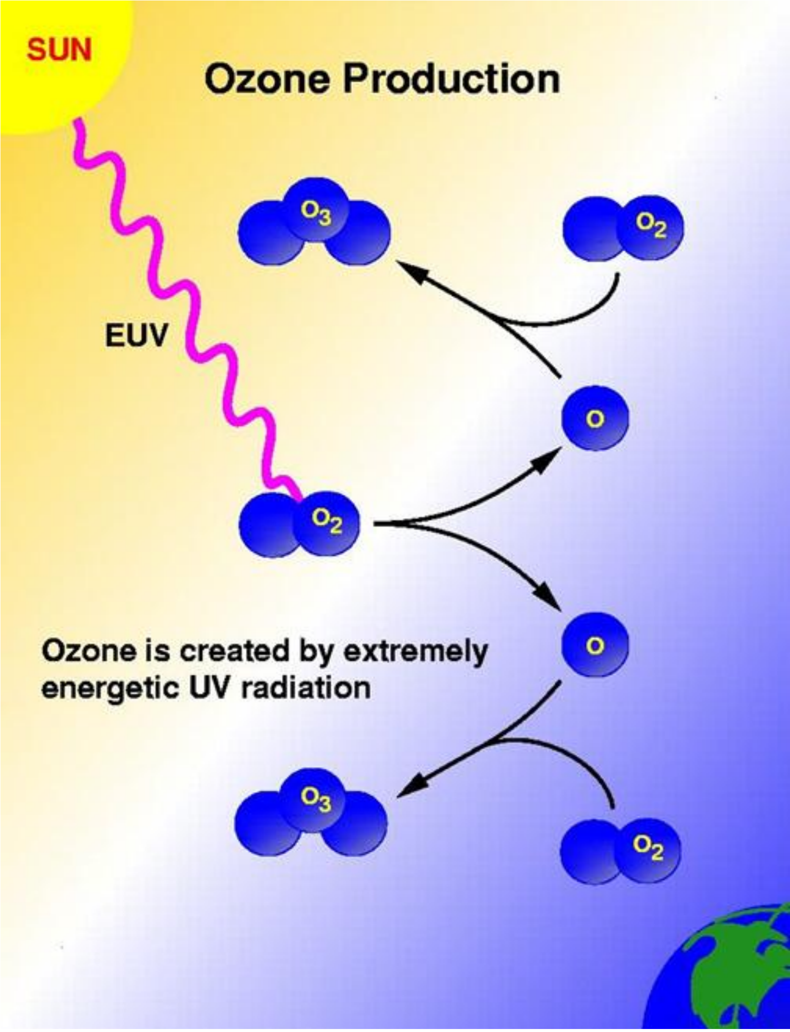


http://lasp.colorado.edu/~bagenal/3720/CLASS5/5Spectroscopy.html

Formación de ozono estratosférico

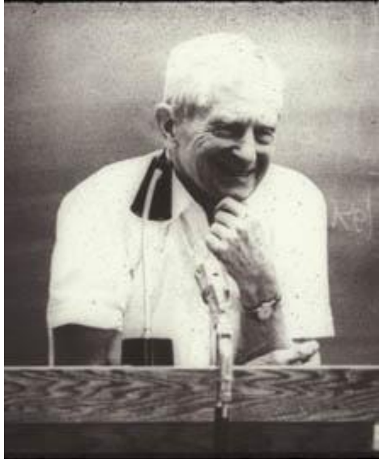


$$O_2 + h\nu \rightarrow O + O, \lambda < 0.24\mu m$$
$$O_2 + O \rightarrow O_3$$



http://www.theozonehole.com/ozonecreation.htm

Ciclo de Chapman



Production:

$O_2 + h\nu$	$\longrightarrow$	$O + O$	$(\lambda < .242\ \mu m)$
$O + O_2 + M$	$\longrightarrow$	$O_3 + M$	

Destruction:

$O_3 + h\nu$	$\longrightarrow$	$O + O_2$	$(\lambda < .320\ \mu m)$
$O + O_3$	$\longrightarrow$	$2\ O_2$	

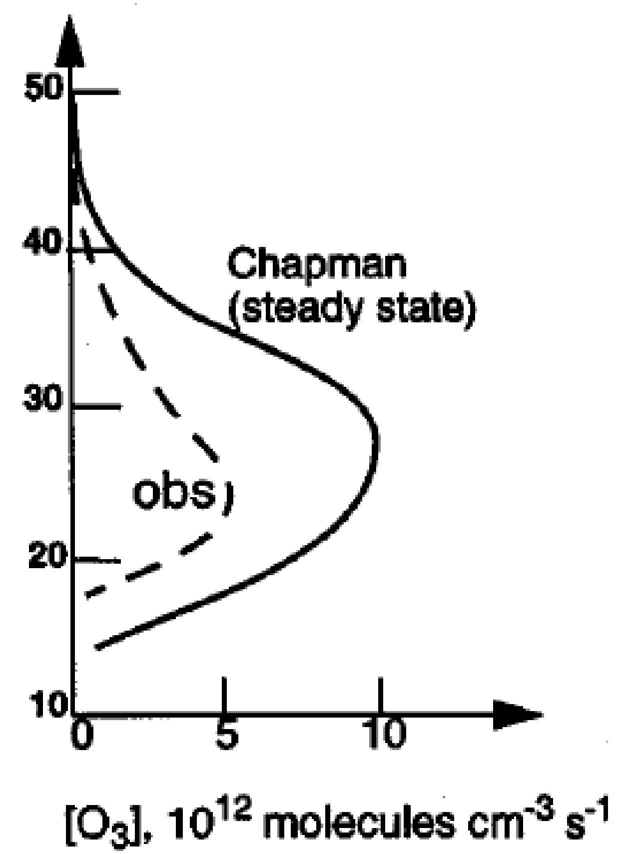
Sydney Chapman, "A Theory of Upper-Atmospheric Ozone," *Memoirs of the Royal Meteorological Society* **3**(26), 103-25 (1930).

¿Qué le faltaba a Chapman?

Ciclos catalíticos de pérdida de ozono:

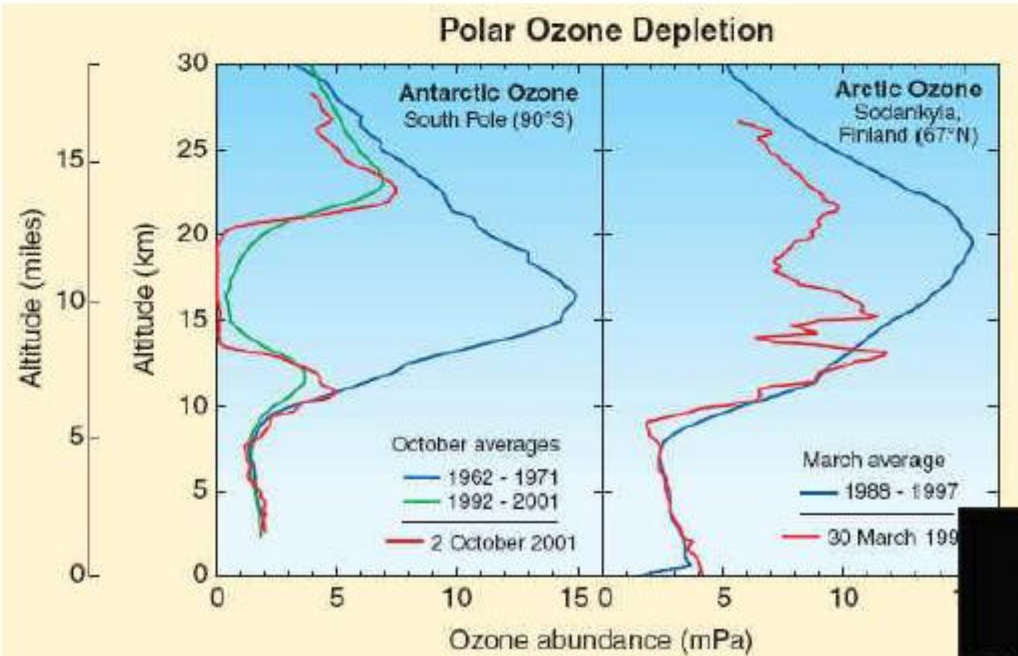
	$X\cdot + O_3$	$\rightarrow$	$XO\cdot + O_2$
	O_3 + *light*	$\rightarrow$	$O + O_2$
	$O + XO\cdot$	$\rightarrow$	$X\cdot + O_2$
net:	$\mathbf{2O_3}$	$\rightarrow$	$\mathbf{3O_2}$

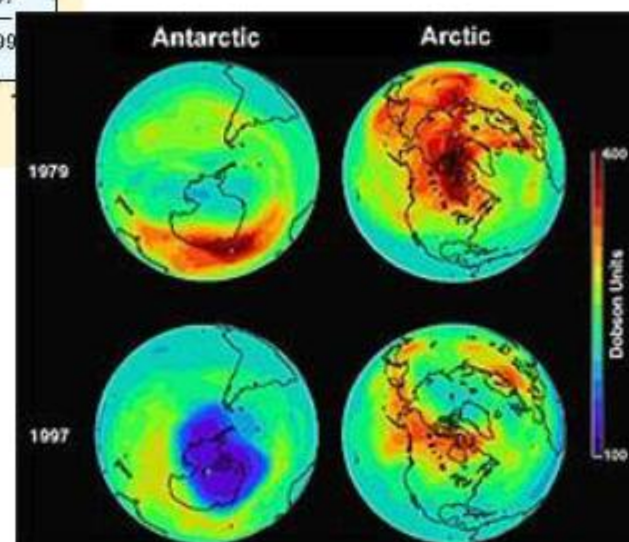
$X\cdot$ = NO, ·OH, Cl; Br·
$XO\cdot$ = NO_2, HO_2, ClO; BrO·



http://www.atmosphere.mpg.de/enid/9605ac397fbcbb857b2468044e746ec2,0/2__Ozone/-_Stratospheric_ozone_208.html

Pero Chapman corregido no explica:



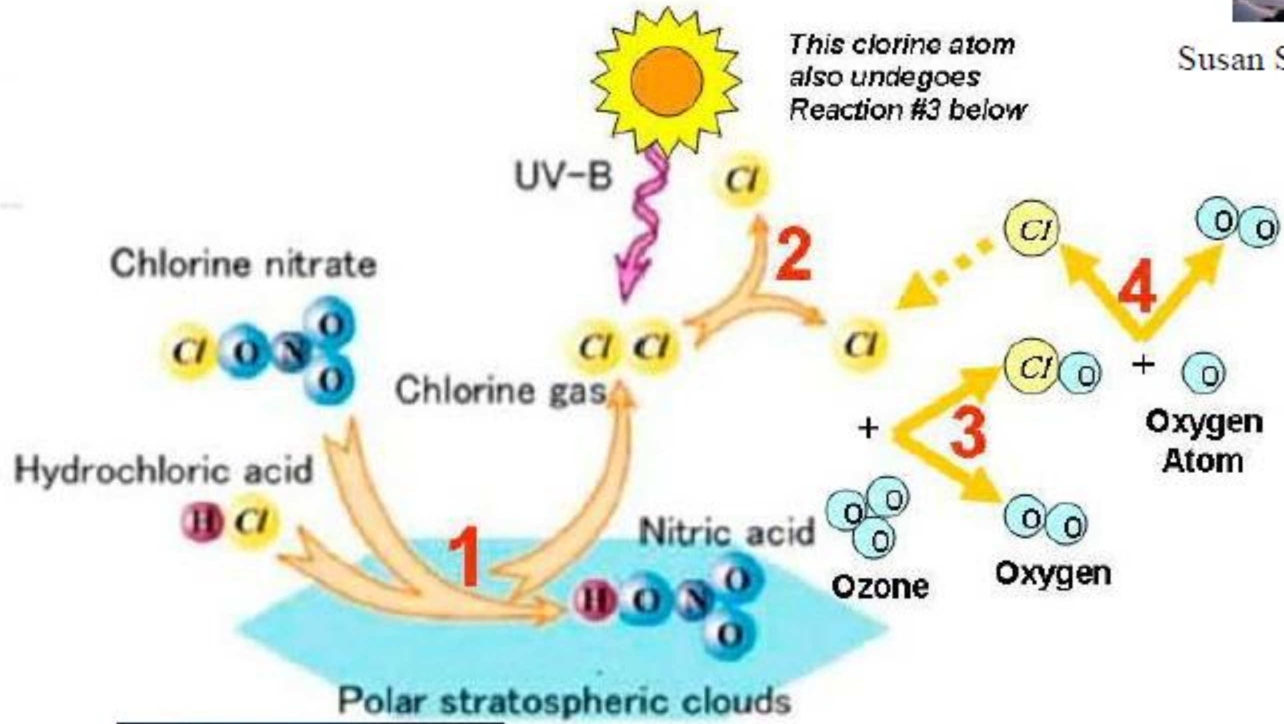


LGK 2011

1 DU=2.69×10^{20} O_3 molec/m^2.

Explicaciones post 1987

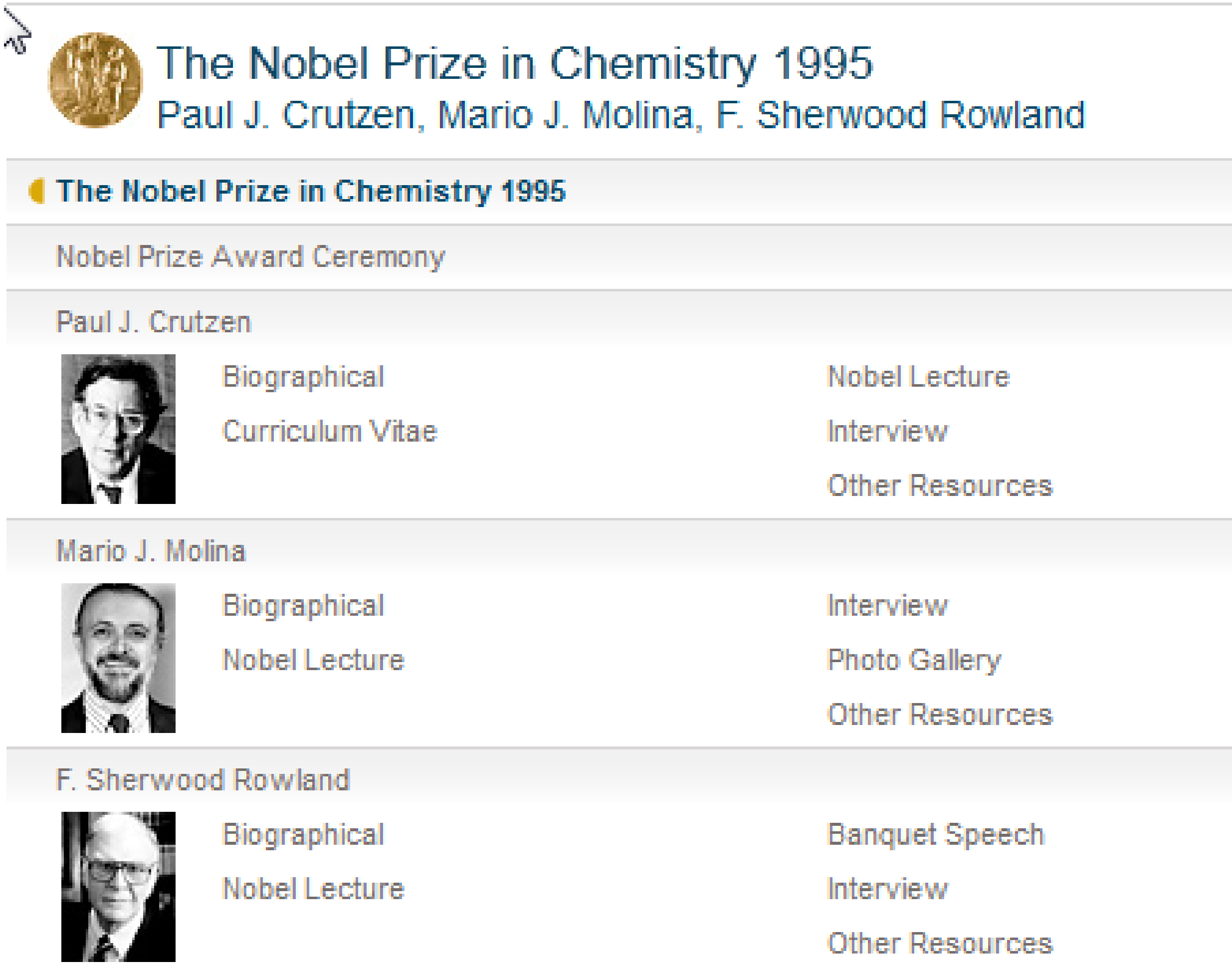
Susan Solomon et al…



LGK 2011

La presencia de nubes polares estratosféricas (PSC) permite reacciones fotoquímicas sobre superficies (más rápidas) que liberan Cl gatillando destrucción de O3. Las PSC son posibles dada la dinámica polar

En Ciencias Atmosféricas hay Premio Nobel


The Nobel Prize in Chemistry 1995
Paul J. Crutzen, Mario J. Molina, F. Sherwood Rowland

The Nobel Prize in Chemistry 1995

Nobel Prize Award Ceremony

Paul J. Crutzen
Biographical
Curriculum Vitae
Nobel Lecture
Interview
Other Resources

Mario J. Molina
Biographical
Nobel Lecture
Interview
Photo Gallery
Other Resources

F. Sherwood Rowland
Biographical
Nobel Lecture
Banquet Speech
Interview
Other Resources

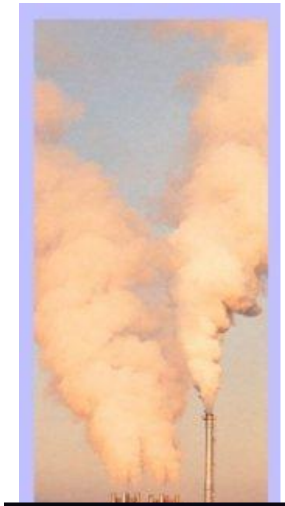
http://www.nobelprize.org/nobel_prizes/chemistry/laureates/1995/press.html#

Pausa (10 minutos)

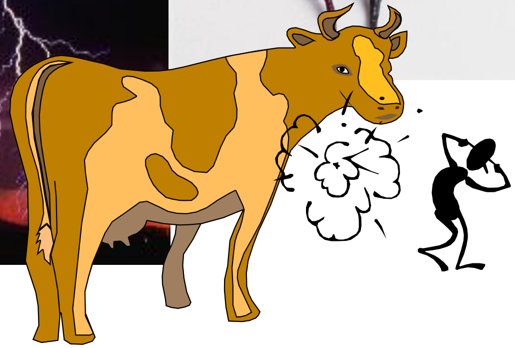
I help you, reach out! Stretch your tiny paw...!

Emisiones

- Emisiones
  - Clasificaciones
  - Inventarios
  - Ejemplos






$$\frac{\partial c}{\partial t} = -\vec{v}.\nabla c - c\nabla.\vec{v} - \nabla.(<c'\vec{v}'>) + Q - S$$

Lavoisier, 1789

+CI & CB

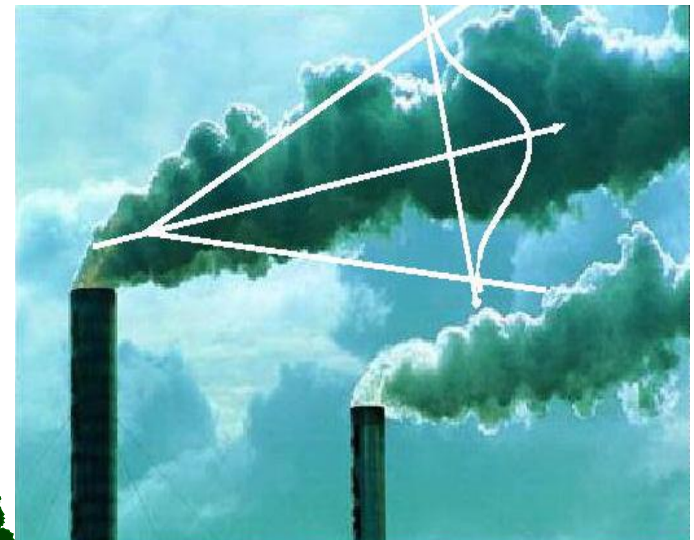
Dispersión y transformaciones

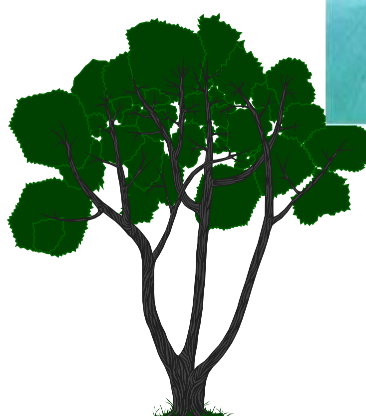
Emisiones

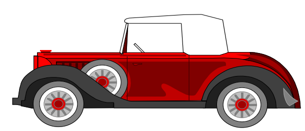
Remoción

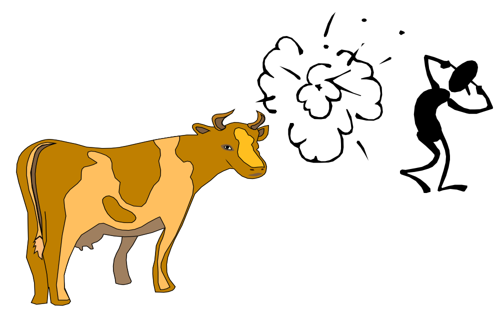
Emisiones

- Qué
- Dónde
- Cuánto
- Cuándo
- Cómo





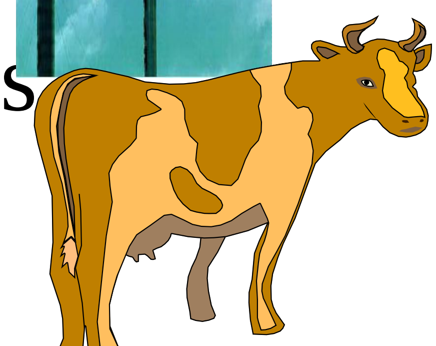


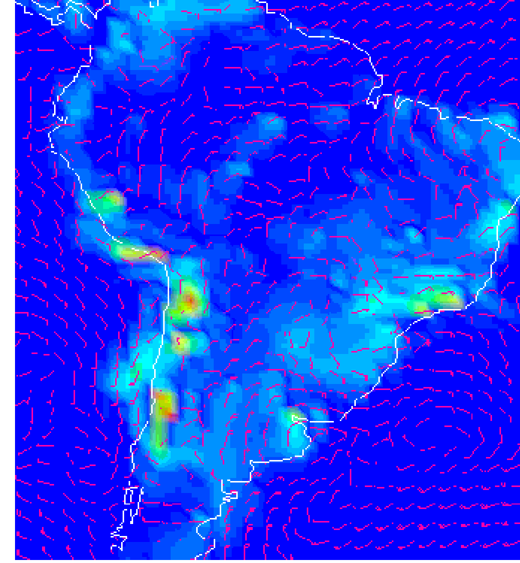


Naturales

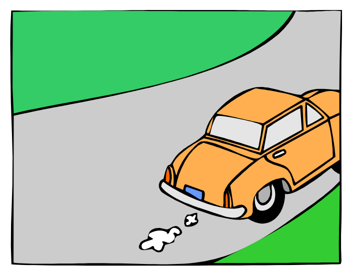
Emisiones

Antrópicas

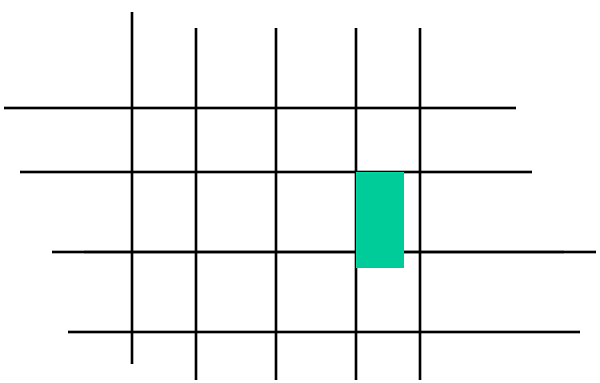




fuente puntual



fuente lineal



fuente superficial

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-- an integrating project of
International Geosphere-Biosphere Program --

brings together

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Input Data Underlying Processes & Inventories
Analysis Tools for Developing & Reviewing Data

to create highest quality
Information Products
on global exchange processes.

GEIA works closely with ACCENT http://www.accent-network.org/
ACCENT Symposium September 12th - 16th 2005 in Urbino, Italy
http://www.accent-network.org/symposium/

Netherlands Environmental Assessment Agency

EDGAR

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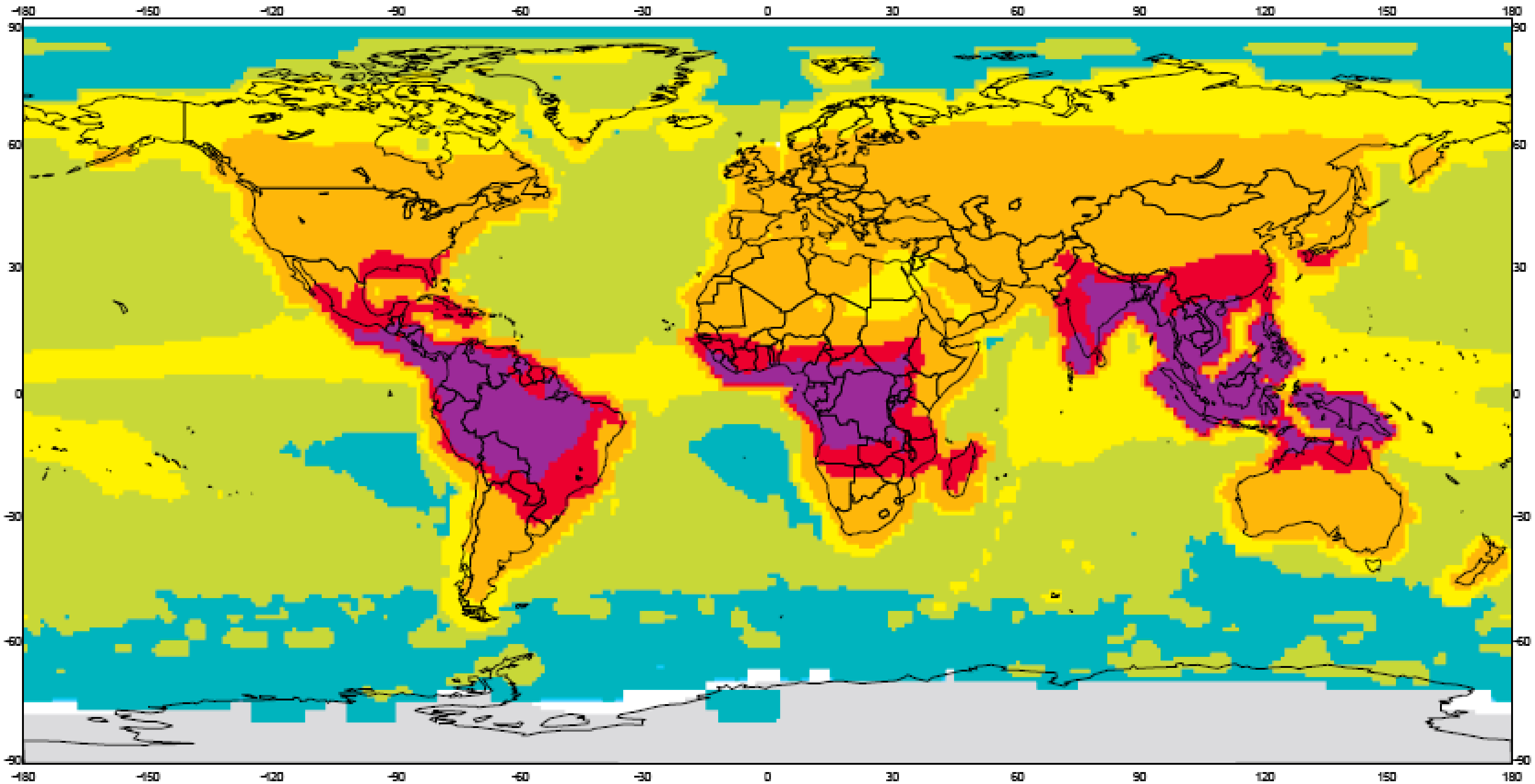
Welcome to the

Emission Database for Global Atmospheric Research (EDGAR)

The EDGAR information system is a joint project of RIVM-MNP, Bilthoven (NL), TNO-MEP, Apeldoorn (NL), JRC-IES, Ispra (IT) and MPIC-AC, Mainz (D), and stores global emission inventories of direct and indirect greenhouse gases from anthropogenic sources including

NO_x from lightning average total (1983 −1990)

Sources: Colin Price, Tel Aviv University, 1997



Global total: 12.2 Tg NO_x-N (min. = 0.1, max. = 4451700)

.

Unit: kg /cell

- 0
- 0 −75
- 75 −750
- 750 −7500
- 7500 −75000
- 75000 −750000
- 750000 −1500000
- 1500000 >

Tangent cylinder projection

.

Theme date: 08/05/98 11:54:36

Note:

8 year average of global NO_x production due to lightning activity.

.

Source: EDGAR

ebDab - Microsoft Internet Explorer

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ción http://webdab.emep.int/ Ir Víncul

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Convention on Long-range Transboundary Air Pollution

emep

Co-operative programme for monitoring and evaluation of the long-range transmissions of air pollutants in Europe

ALL
EU15
EU18
EU25
———

2030
2025
2020
2015
2010

Pollutants

Main Pollutants	Heavy Metals	POP	PM
ALL	ALL	ALL	ALL
———	———	———	———
CO	As	Aldrin	PM10
NH3	Cd	Chlordan	PM2.5
NMVOC	Cr	Chlordecone	TSP

Emission Category

[NFR02 / Guidelines 2002]
National Total
Legislation Projection Total
Reduction Projection Total
NFR02 (level1)

Sectors (optional)

[NFR02 (level 1)]
N02 01 – Combustion in Power Plants and Industry
N02 02a – Transport above 1000m
N02 02b – Transport below 1000m
N02 03 – Commercial, Residential and Other Stationary Combus

☑ Include Report Information & Footnotes

Latest Year of Reporting: 2006

Type and Format

HTML Table Options

Official Emissions Activity Data Expert Emissions User Guide Intro Page

Internet

Factores de emisión: simples pero muy complejos

$E = A \times EF \times (1 - ER/100)$

donde:

- E = emisión;
- A = tasa de actividad;
- EF = factor de emisión
- ER =factor de eficiencia %

Factores de Emisión

$$E = k * 1.7 * \frac{s}{12} * \frac{S}{48} * \left(\frac{W}{2.7}\right)^{0.7} * \left(\frac{w}{4}\right)^{0.5} * \left(1 - \frac{p}{365}\right)$$

•E: factor de emisión (kg de polvo emitidos por vehículo y km transitado

•k:coef. de tamaño de partícula emitida

Tamaño (μm)	Ω30	Ω15	Ω10	Ω5	Ω2.5
k	0.80	0.50	0.36	0.20	0.095

•s: contenido de finos en %

•S: velocidad media de circulación en km/hr

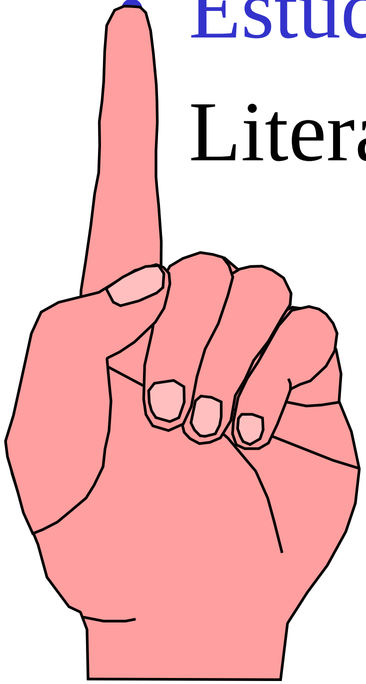
•W: peso medio de los vehículos en toneladas

•w: número de ruedas

•p: número de días con precipitación
mayor o igual a 0.254 mm

¿Dónde se consiguen?

- Agencias ambientales extranjeras. Por ejemplo “AP 42 EPA” (http://www.epa.gov/ttn/chief/index.html)
- Estudios propios (Ver estudios DIMEC)
- Literatura



¿Aplicabilidad?

Incertidumbre

Estudios de sensibilidad

vo Editar Ver Historial Marcadores Herramientas Ayuda

US EPA http://www.epa.gov/ttn/chief/index.html

Google

U.S. Environmental Protection Agency

Technology Transfer Network
Clearinghouse for Inventories & Emissions Factors

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Emissions Inventories

Emissions Inventories are the basis for numerous efforts including trends analysis, regional, and local scale air quality modeling, regulatory impact assessments, and human exposure modeling.

Emissions Factors

The Emissions Factors & Policy Applications Center (EFPAC) provides information about existing emission factors, the revision of existing factors and the development of new factors from stationary point and non point sources.

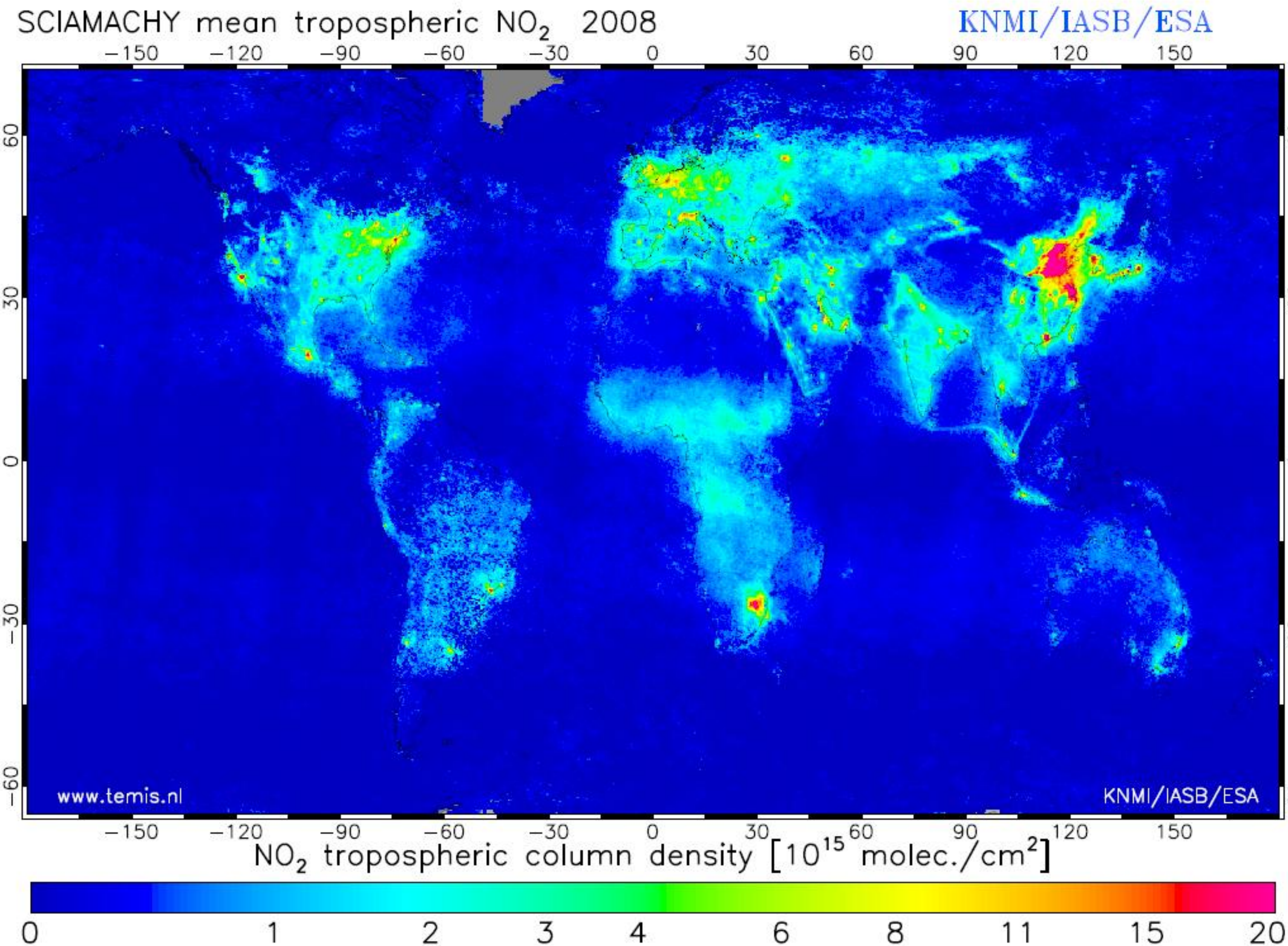
Emissions Modeling

The Emissions Modeling Clearinghouse (EMCH) has been designed to support and promote emission modeling activities both internal and external to the EPA. Through this site the EPA intends to distribute emissions model input formatted inventories based on the latest versions of its National Emission Inventory databases.

Emissions Monitoring Knowledge Base

EPA's Monitoring Knowledge Base Site provides information about monitoring techniques for air pollution control. The monitoring information is presented by industry type and by control technique.

	CO_2 Pg C yr^{-1}	CH_4 Tg CH_4 yr^{-1}	N_2O Tg N yr^{-1}	Sulphur Tg S yr^{-1}	NO_x Tg N yr^{-1}	CO Tg CO yr^{-1}
Natural	150*	160	10.2	18	11	200-600
Human-related						
Fossil fuel and industry	6.8	100	1.3	65	22	300-500
Biomass burning	1.6*	40	0.5	2	12	300-700
Agriculture		170	3.9		1	
Landfills/sewage		65				
Other						300-800
Human total, present	7.6	375	5.7	67	35	900-2000
Human-related, 2100**	3.3-36.8	236-1069	4.8-19.3	11-69	16-110	363-3766

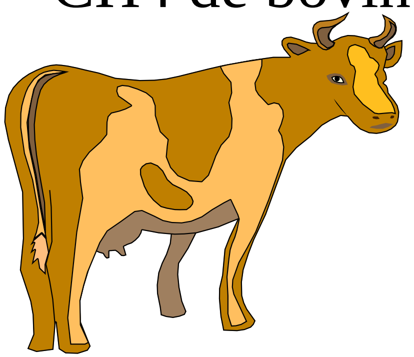

SCIAMACHY mean tropospheric NO_2 2008
KNMI/IASB/ESA
−150 −120 −90 −60 −30 0 30 60 90 120 150
60 30 0 −30 −60
www.temis.nl
KNMI/IASB/ESA
NO_2 tropospheric column density [10^{15} molec./cm^2]
0 1 2 3 4 6 8 11 15 20

¿Cómo hacer un inventario de emisiones?

CO vehicular en Santiago

NOx en descargas eléctricas

CH4 de bovinos



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