ATMOSPHERIC DYNAMICS

from the bottom up:-

microscale → mesoscale →macroscale

10^{-10} m < 10^{-6} m < 10^{-5}m and up

Turbulence: Vertical Shear of the Horizontal Wind, Jet Streams, Symmetry Breaking, Scale Invariance and Gibbs Free Energy. *Atmosphere,* **12,** 1414 (2021).

KEY POINTS [1]

* Connection between microscopic and macroscopic processes
    * Emergence of organized flow in a randomized (thermal) gas
    * Persistence of molecular velocity after collision
    * Symmetry breaking, of continuous translational symmetry
* Existence of scale invariance in atmospheric observations
    * Aircraft: ER-2 & WB57F lower stratosphere / DC-8 & G4SP upper troposphere
    * GPS dropsondes: 13 km to surface of Pacific Ocean
* Correlations with & among scaling exponents: H, C_1 and α
    * Intermittency C_1 of temperature and $J[O_3]$
    * Scaling of wind & temperature H with jet gradients
    * Correlation of H and α for ozone inside polar vortex

KEY POINTS [2]

* **Implications from scaling exponents**

    * **Sources and sinks from scaling exponents**

    * **23/9 dimensionality and Law of Mass Action**

* **Entropy and Gibbs free energy from scaling**

    * **Thermodynamics, steady states**

    * **Vertical scaling of temperature and model cold bias**

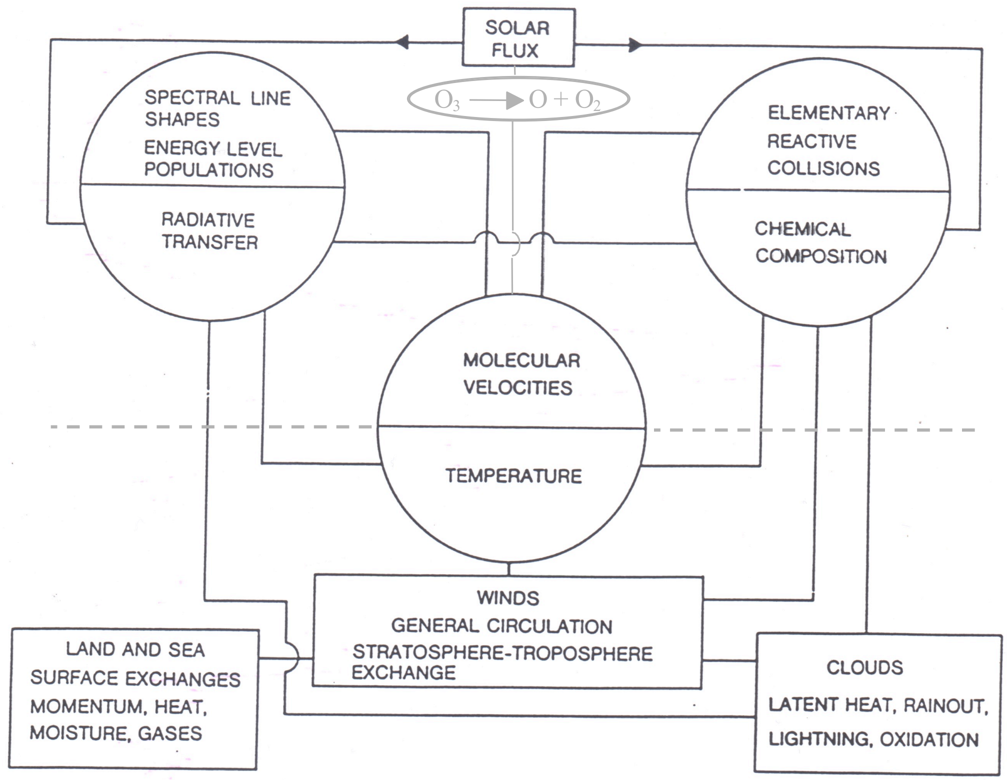
    * **Overpopulation of fast molecules in air**

* **Multifractal scaling exponents**

H, C_1 and α **Conservation, intermittency and Lévy**

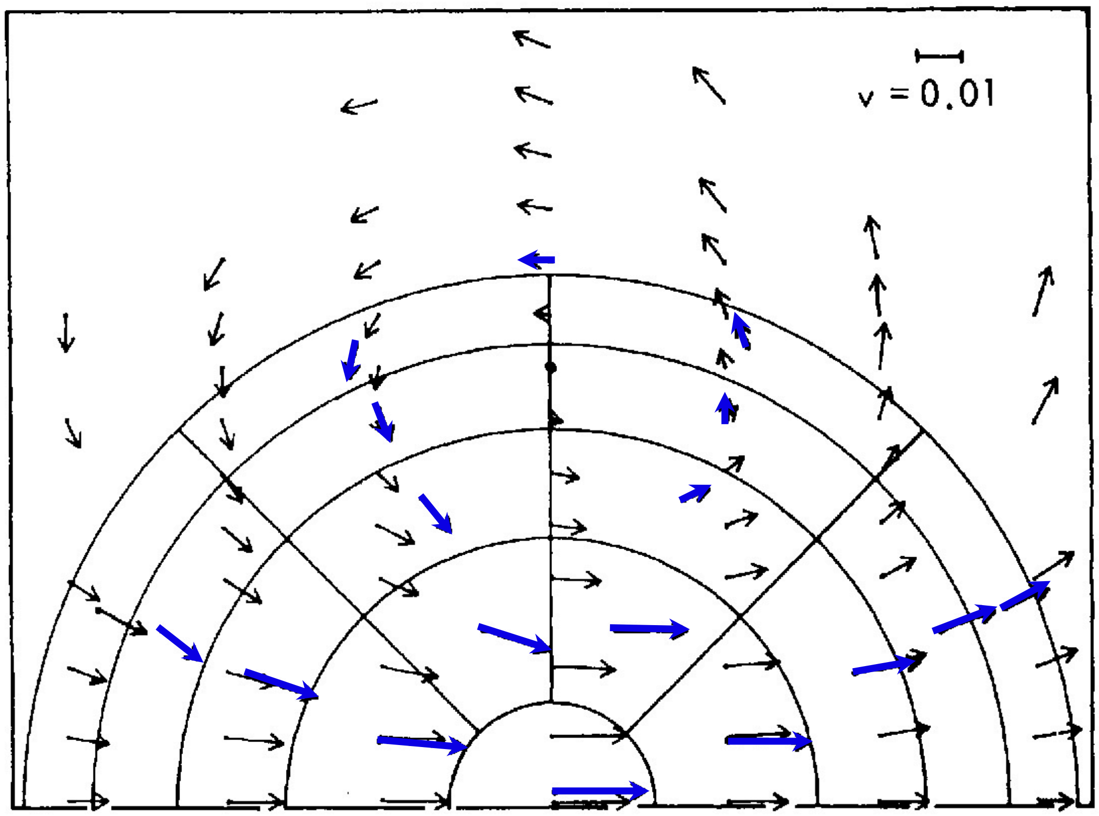
Slide 2

The correspondence and coupling of the microscopic and macroscopic processes in the atmosphere.



Slide 3

Alder & Wainwright (1970): molecular dynamics simulation of a flux applied to an equilibrated Maxwellian population results in the emergence of vortices on scales of 10^{-12} seconds & 10^{-8} metres.



Equivalence between statistical thermodynamic and scaling variables.

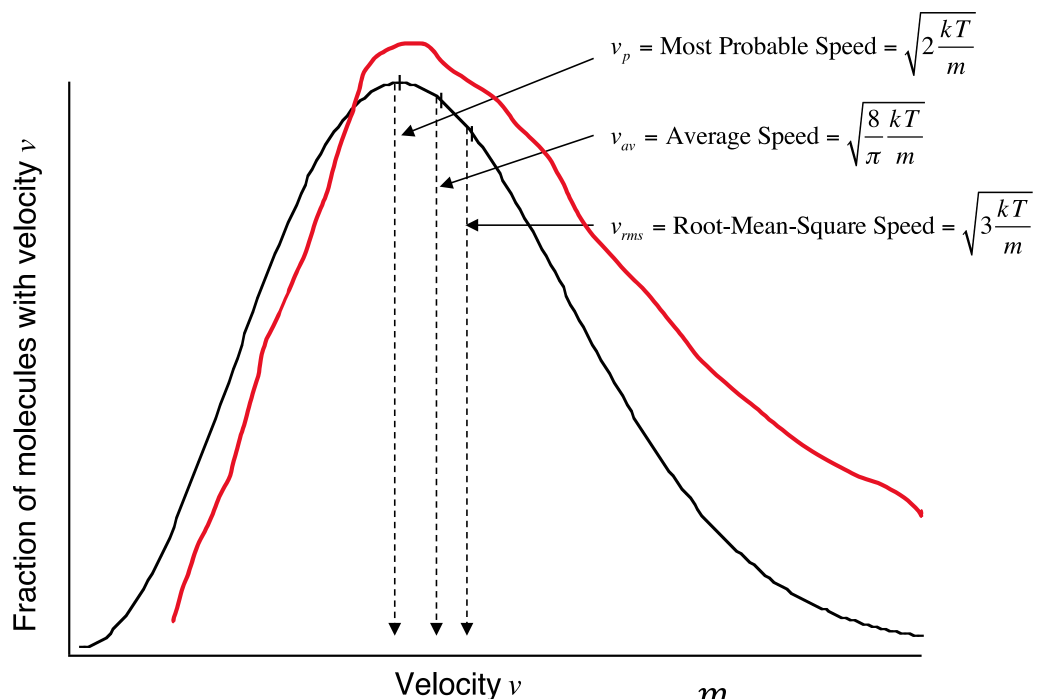
Variable	Statistical thermodynamics	Scaling equivalent
Temperature	T	$1/qk_{Boltzmann}$
Partition function	f	$e^{-K(q)}$
Energy	E	γ
Entropy	-S(E)	$c(\gamma)$
Gibbs free energy	-G	K(q)/q

Slide 5

Maxwellian Velocity Distribution

“Observed” or “MD calculation”

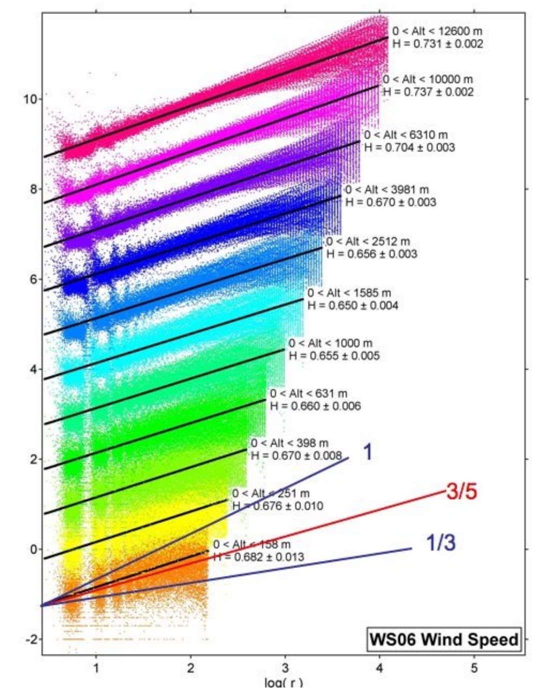
$$\frac{N_V(v)}{N} = 4\pi\left(\frac{m}{2\pi kT}\right)^{\frac{3}{2}} v^2 e^{-\frac{KE}{kT}}$$



$$T = \frac{m}{3k}\langle(v - \langle v\rangle)^2\rangle$$

Slide 6

Vertical Scaling of the Horizontal Wind, GPS Dropsondes from 13 km to surface of Pacific Ocean, (21-60N,128-172W)



Slide 7

Persistence of molecular velocity after collision

$$w_{12} = \frac{1}{2}m_1 + \frac{1}{2}m_1^2 m_2^{-1/2}\ln[(\sqrt{m_2} + 1)/\sqrt{m_1}]$$

$w_{12} = 0.406$ if $m_1 = m_2$, otherwise heavier molecule slows less

Thermal wind equation - meteorology

$$\partial \boldsymbol{V}_{\mathbf{g}}/\partial \mathrm{z} = (g/fT)\mathbf{k}\times\nabla_{\mathbf{p}}T$$

As altitude above tropopause increases, g decreases and T increases

Barometric equation – physical chemistry

$$\ln(\mathrm{C}_2/\mathrm{C}_1) = \mathrm{N}_0\mathrm{mg/RT}(z_1 - z_2)$$

As altitude above tropopause increases, g decreases and T increases

Slide 8

Emergence of organized flow in a randomized gas

* Production of vorticity at scale of molecular mean free path.

* Anisotropy ubiquitous in air.

* No local thermodynamic equilibrium, no isotropic diffusion.

* Fastest molecules cause flow, average ones define temperature.

* Opposite of conventional meteorological decomposition into an organized mean and dissipative eddies (Langevin equation).

* Red PDF velocity – black (Maxwellian) PDF velocity → Gibbs free energy .

* “Gibbs molecules” break continuous translational symmetry by persistence of velocity after collision.

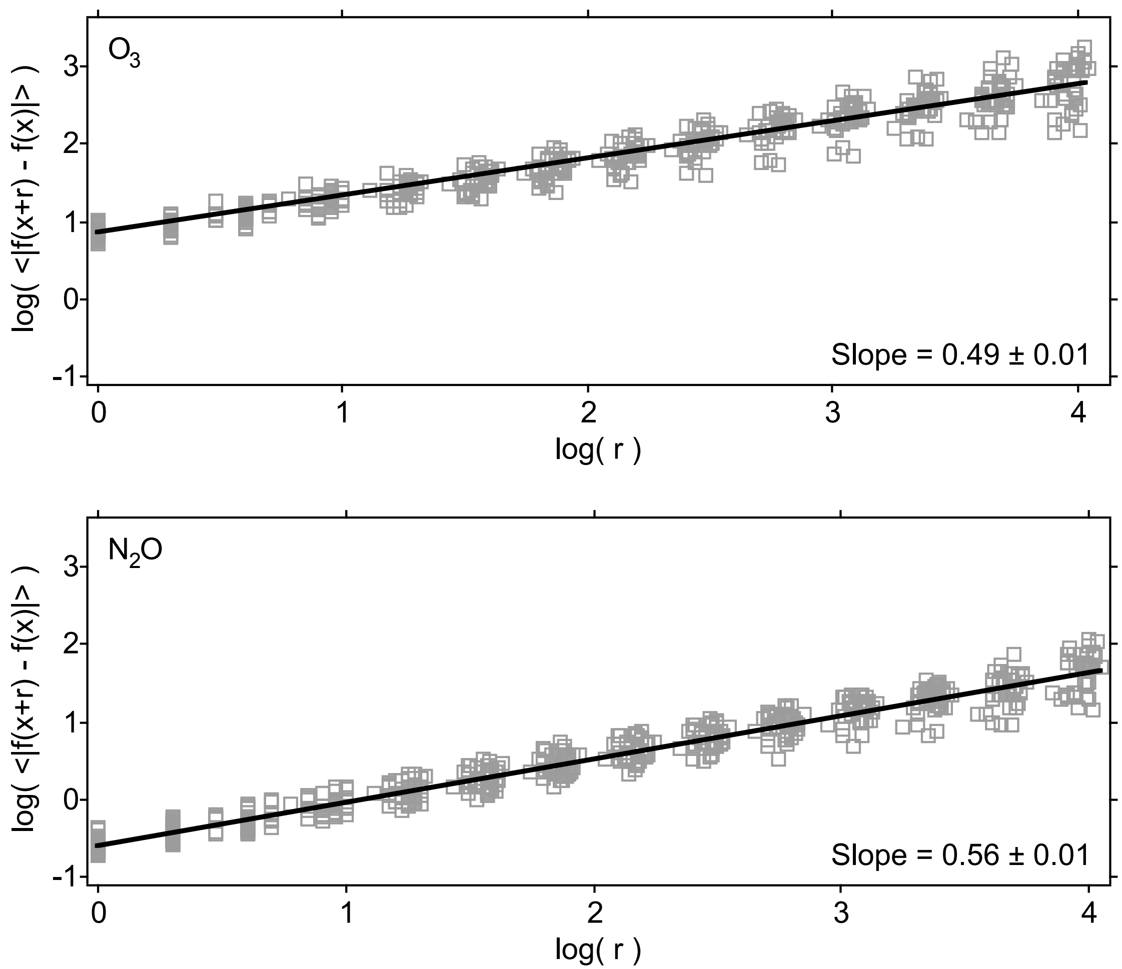
What to do about it?

* Molecular dynamics simulation of stratospheric air.

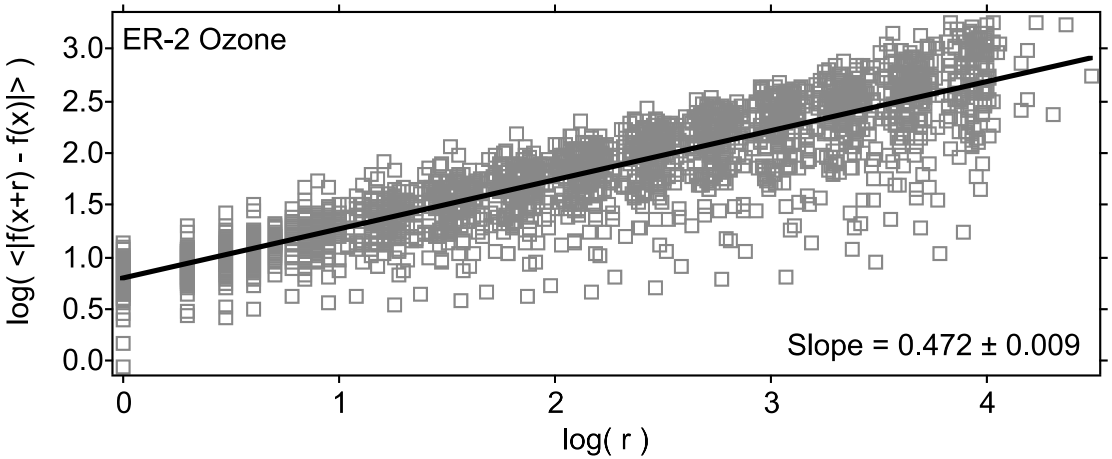
* Experimental tests of better atmospheric observations.

* Develop better model formulations, dynamically, chemically and radiatively.

All ER-2 ozone & nitrous oxide, 59˚N-70˚S, heavy SH weighting



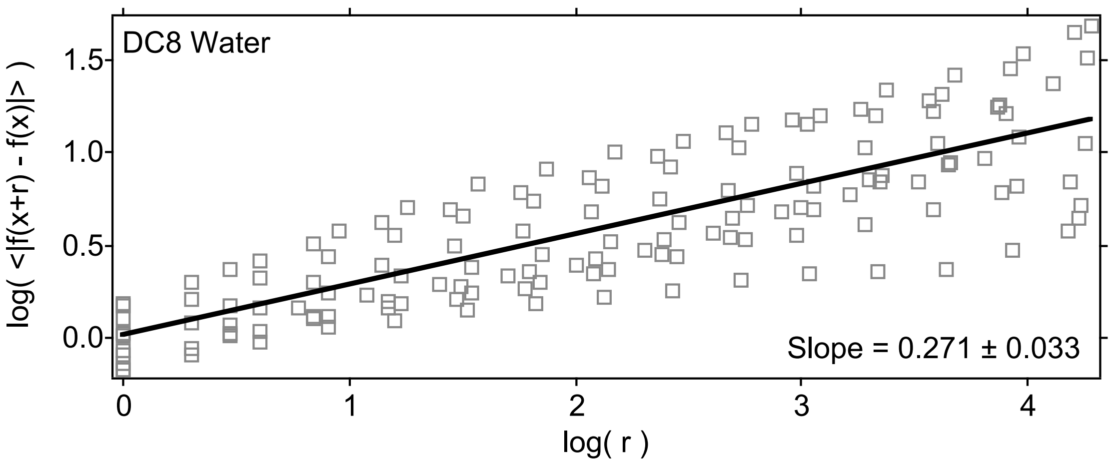
All ER-2 'horizontal' segments >2000 s, 1987-2000



O_3 sink in polar vortex: H < 5/9

Slide 11

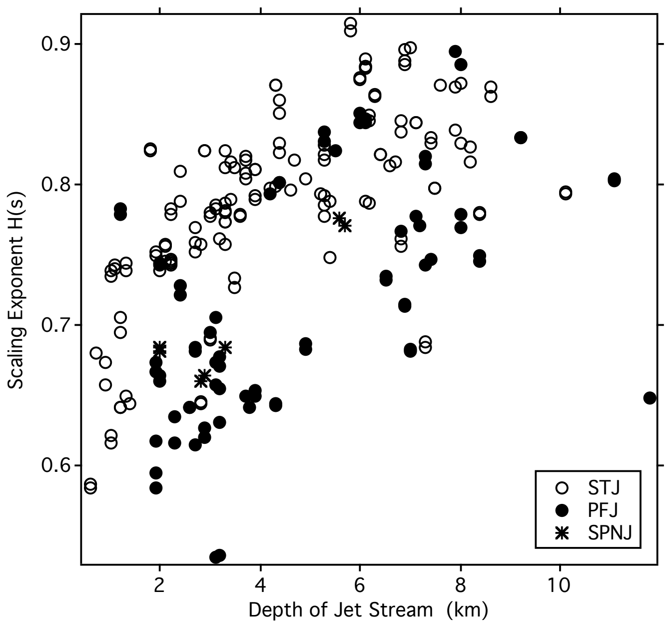
All DC-8 total water, 'horizontal', 44˚S - 90˚S, Aug-Sep 1987

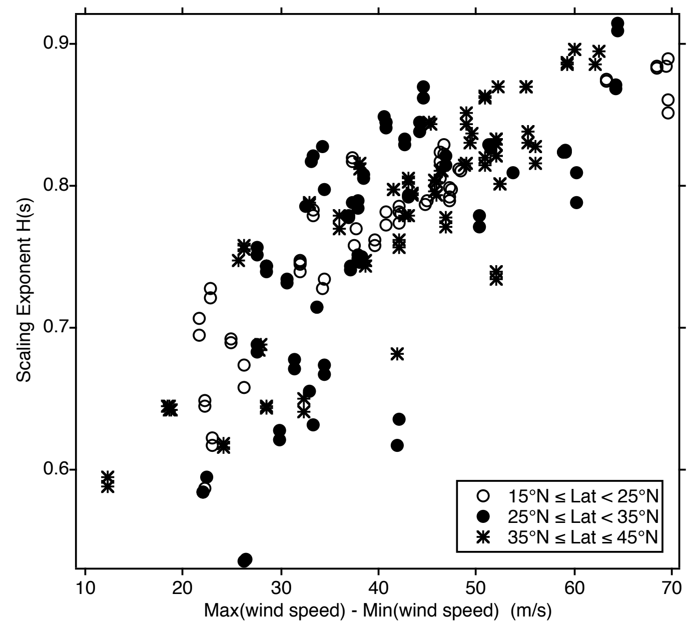


H < 5/9 indicates a sink is operative - gravitational settling of ice

Slide 12

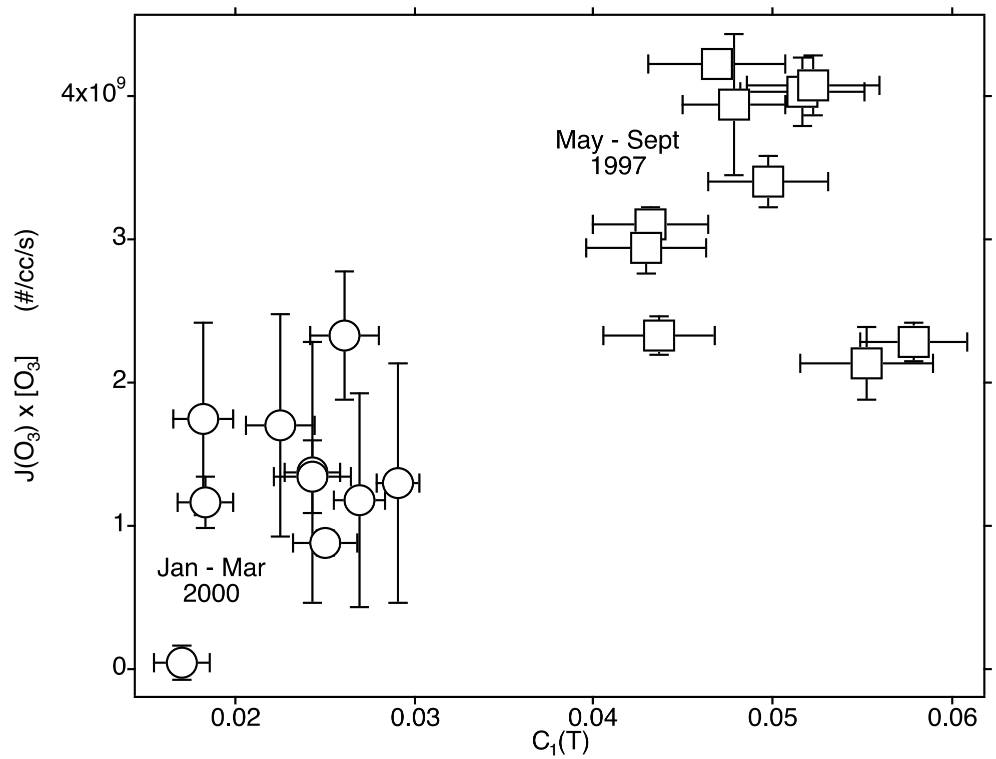
Correlation of *H* for dropsonde wind speed with jet strength, WS 2004





Slide 13

Correlation of the observed photodissociation rate of ozone with the intermittency of observed temperature. Arctic summer 1997 and winter 2000.



Overpopulation of high-speed molecules relative to Maxwell-Boltzmann

* Effect on spectroscopic line shapes in wings and hence radiative transfer.

* Effect on temperature, especially in upper stratosphere. [model cold bias?]

* Effect on chemical kinetics.

What to do about it?

* Experiments, e.g. vary [O_3] and [H_2O] with and without ozone photodissociation while taking high resolution spectra.

* Molecular beam experiments with velocity PDF measurement in air - difficult!

* See if translationally hot $O(^3P)$ atoms accelerate atmospheric chemistry. Do they scramble isotope fractionation?

* Effect should accelerate reactions with an activation energy, and decelerate those with a negative temperature dependence, e.g. radical - radical recombinations.

* Molecular dynamics calculations: could cover lowest 3-4 decades of scale.