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Tutorial Lecture #6

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Physics and Chemistry of the Mesopause Region

Physics and Chemistry of the Mesopause Region

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- Processes involved in the coupling between composition, energy and dynamics

- Importance of external forcing

Outline

- composition of the mesopause region: how it differs from other regions

- impact of dynamics and energy on composition

- impact of composition on energy and dynamics

- example: role of CO_2 in mesopause structure

- example: photochemical destabilization of gravity waves

Definitions

- mesopause: altitude of the temperature minimum, which varies on seasonal and shorter time scales; the talk will consider the range 80-100 km.

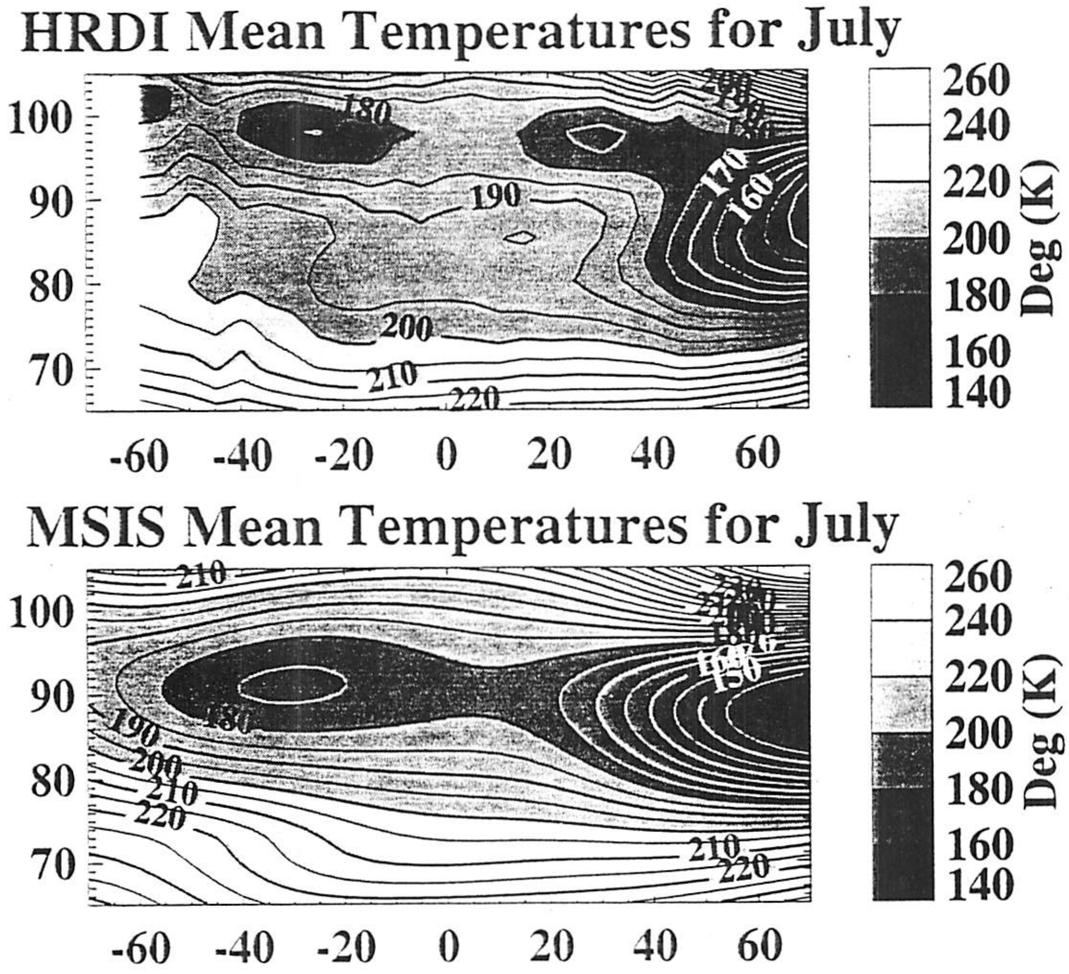
- composition: mostly concerned with the variable part of the composition, making up $\leq$1% of the total

- mixing ratio: density of species/total density

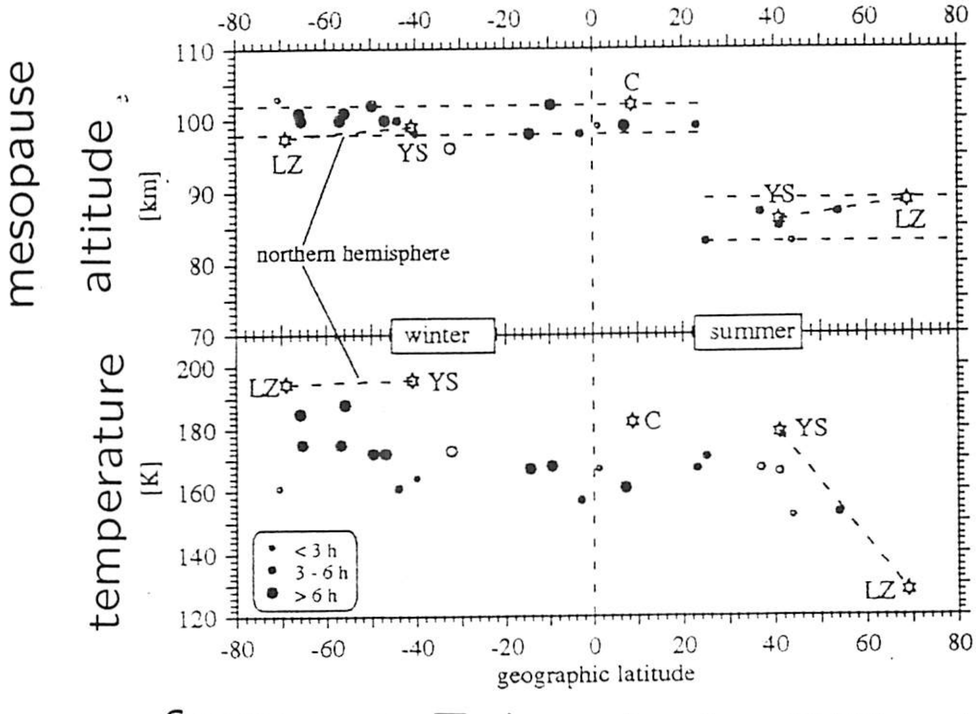
- energetics: the thermal budget & the processes for converting between heat and other forms of energy

- vertical scale: for the models, log(pressure) scaled to give approximate altitude

Note: many of the illustrations are taken from numerical models



from Ortland et al., *JGR*, 1998



from von Zahn et al., *GRL*, 1996

Which atoms & molecules are present?

THERMOSPHERE

- decrease in proportion of dominant molecules (O_2, N_2)
- increase in several simple molecules (NO, CO)
- increasing dominance of atoms
- more excited states
- reactions can be slow because of low density
- ions and ion reactions are important

STRATOSPHERE & LOWER MESOSPHERE

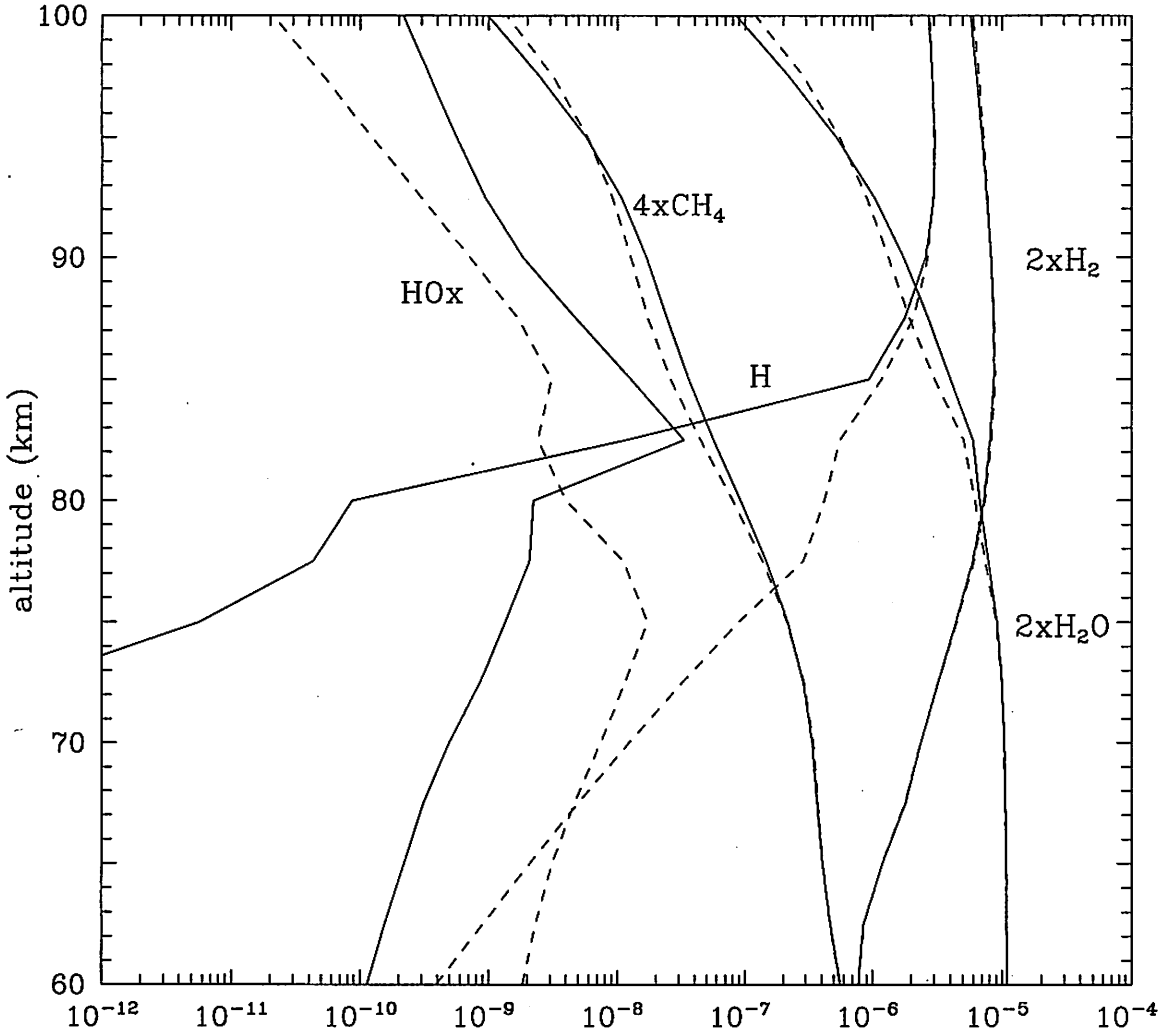
- breakdown of larger molecules produced in the troposphere
- larger role for atoms than in the troposphere
- density is still high enough for 3-body reactions
- sharp daytime maximum of some atoms & compounds (O, Cl, H, OH, NO, etc.)
- only one excited species ($O(^1D)$) plays a significant role
- catalytic cycles of NOx, ClOx and HOx destroy ozone

Which atoms & molecules are present?

UPPER MESOSPHERE

- dominant molecules (O_2, N_2) still well mixed
- concentrations of NO, CO can be large
- excited states participate in chemistry ($N(^2D)$) or energetics (e.g., $O_2(^1\Sigma)$)
- a few tropospheric molecules remain: H_2O, CO_2
- increasing role for atoms, particularly O and H
- decreasing density affects 3-body reactions
- photochemically driven diurnal variations of most minor species
- catalytic cycle of HOx dominates ozone destruction
- ions (NO+) begin to have an effect on neutrals

Compounds containing H



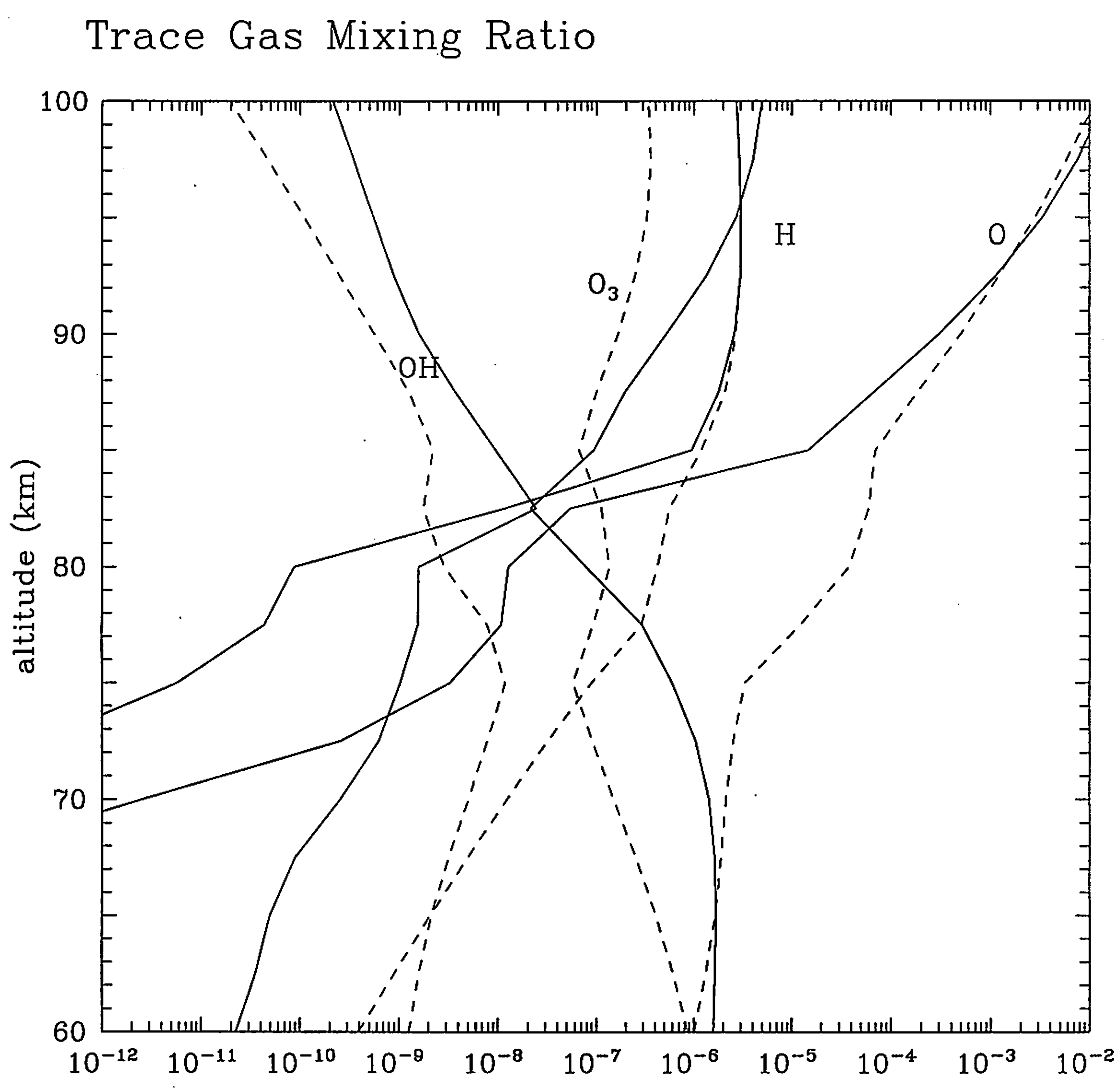
What are the important species?

1) from the point of view of controlling the composition:

- O: produced locally from O_2 and O_3, transported downward from thermosphere; increases strongly with altitude
- O_3: produced from $O+O_2$; rapidly destroyed during the day
- H, OH, HO_2: produced during the day from H_2O, or transported downward from thermosphere (H)

2) from the point of view of measurements

- O_3
- CO_2
- sodium and other metals
- excited species that emit: $O_2(^1\Sigma)$, OH, etc.



Trace Gas Mixing Ratio
altitude (km)
100
90
80
70
60
10^{-12}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
OH
O_3
H
O

Which reactions occur?

photolysis, e.g: $O_3 + h\nu \rightarrow O + O_2$

- sun angle
- solar flux
- column of absorbing gases
- weakly on temperature

2-body reactions, e.g: $O + O_3 \rightarrow O_2 + O_2$

- density of reactants
- temperature

3-body reactions, e.g: $O + O + M \rightarrow O_2 + M$

- density of reactants
- temperature
- density

*M is any atom or molecule

Day/Night Differences

Daytime

- Sunlight splits molecules: O_2, O_3, H_2O
- Absorption generates excited states of atoms and molecules that can react chemically or pass their energy along to another species

Nighttime

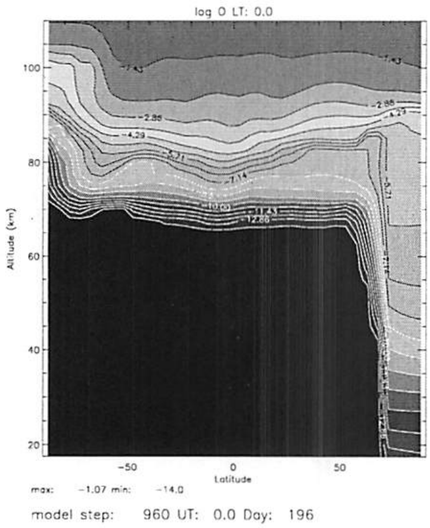
- at lower altitudes atoms & radicals recombine into more stable molecules (e.g., $O \rightarrow O_2$, O_3 and H, OH, $HO_2 \rightarrow H_2O$
- O and H persist at the mesopause & above

Transport

- dynamics is similar except for phase of the tides & processes affected by tides
- vertical transport can be very different because of gradients

Global log(mixing ratio) of O at four local times

0 LT



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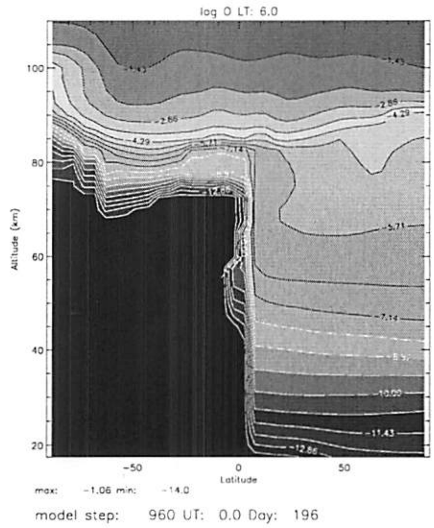
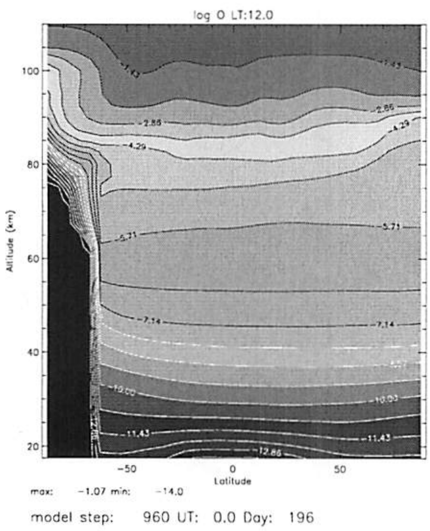
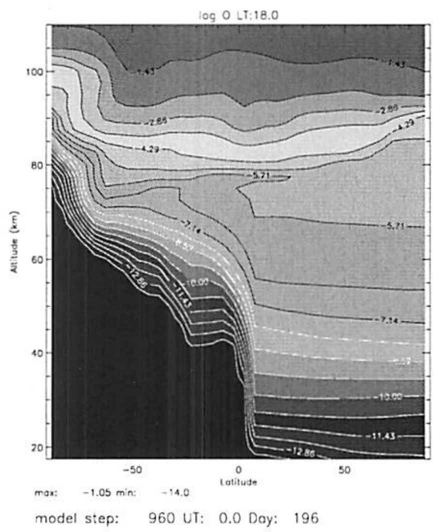


12 LT



18 LT



Impact of anthropogenic gases on composition

- increased CO_2 → cooling
- increased hydrocarbons → ozone loss

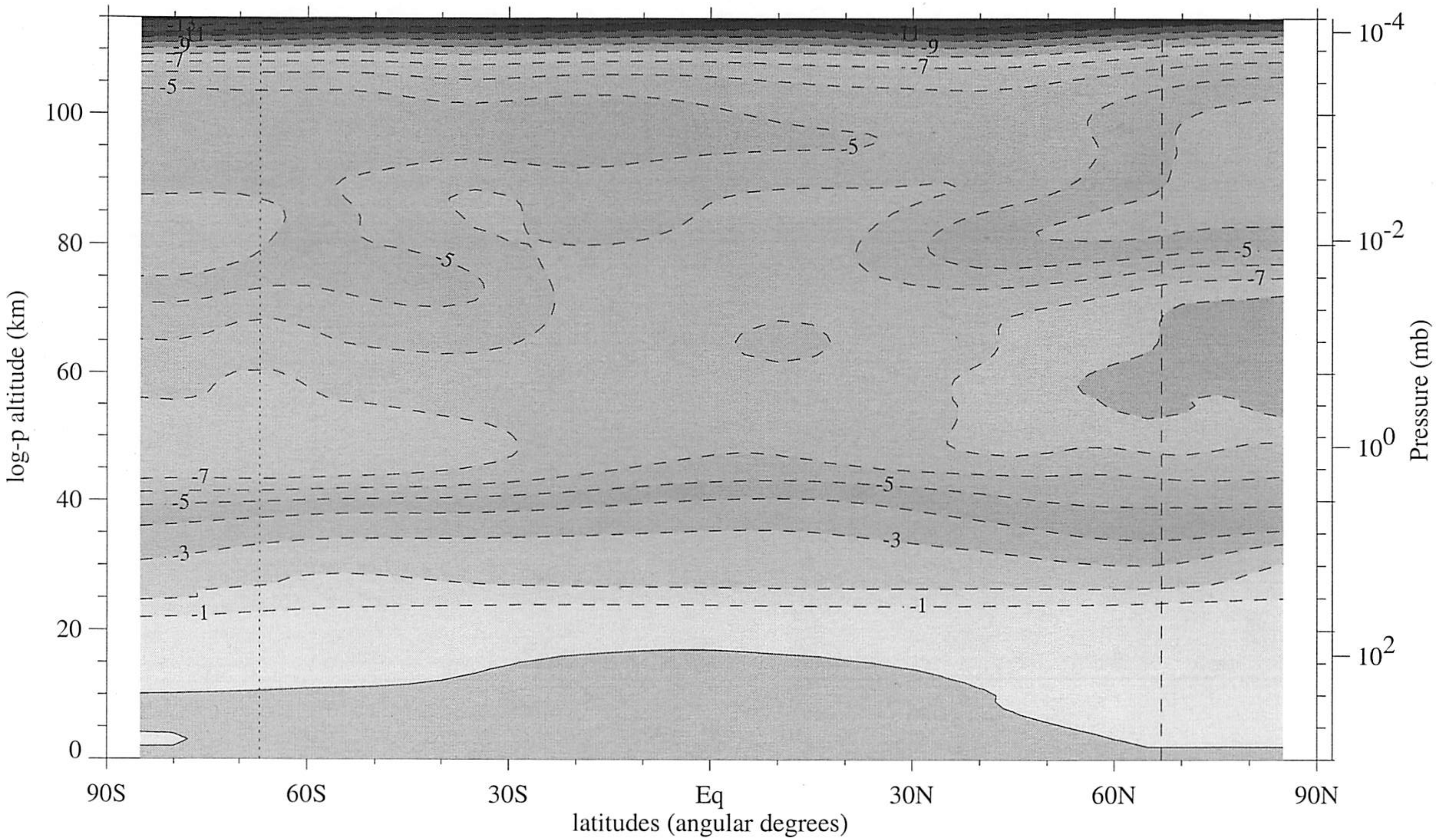
Impact of dynamics on composition

- winds advect species
- temperature affects reaction rates
- winds and temperature control propagation and dissipation of waves

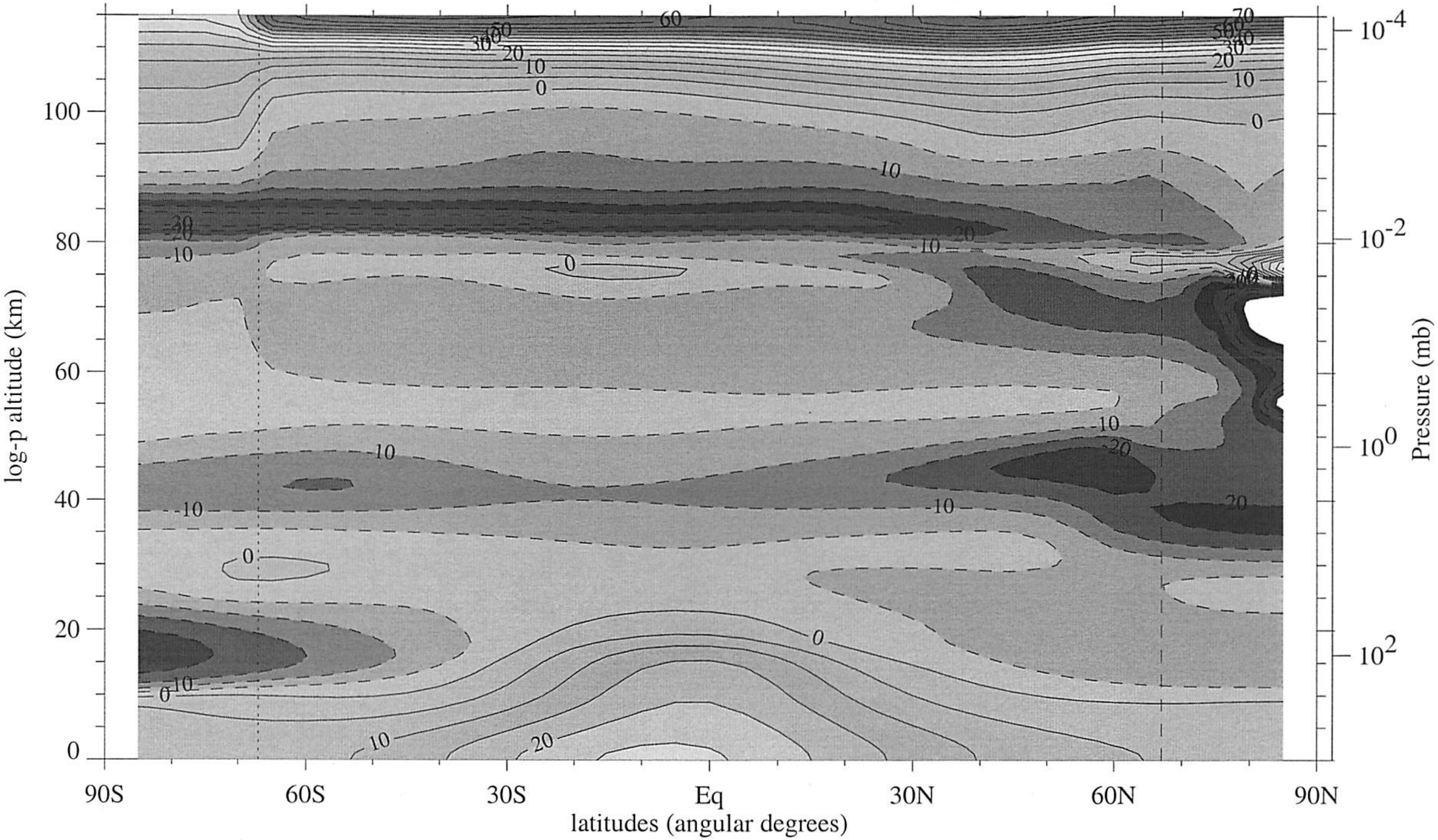
Impact of energetics on composition

- photolysis affected by incident radiative flux
- atomic/molecular energy levels changed by absorption of radiation
- energetic particles can generate ionized or excited states
- temperature affects reaction rates

temperature ABSOLUTE DIFFERENCE (K)



O_3 relative difference (%)



Diffusive transport

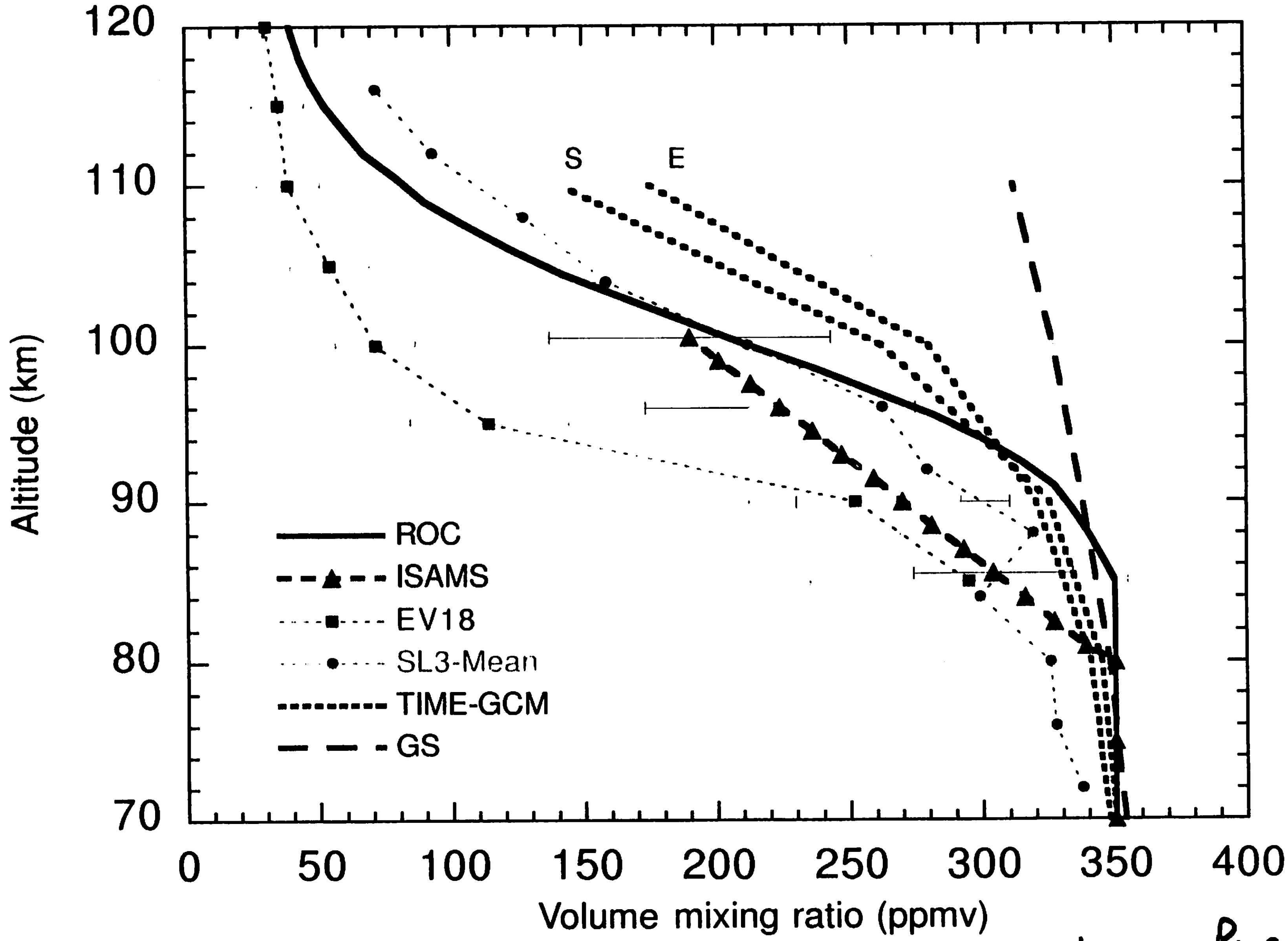
molecular diffusion

- diffusive component reduces gradients
- "advective" component moves species differentially
- effects on mesopause H, H_2, CO_2, temperature
- diffusion rate varies with temperature

eddy diffusion

- caused by turbulence or by any unresolved dynamical scales
- important in the vertical because of strong mixing ratio gradients
- limited measurements
- mass mixing, i.e., all species (mixing ratio) and potential temperature have same diffusion coefficient
- extremely variable due to intermittent dynamics

Fig. 5. Comparison of measured and calculated CO_2 mixing ratios



Lopez Puertas et al.

Advective transport

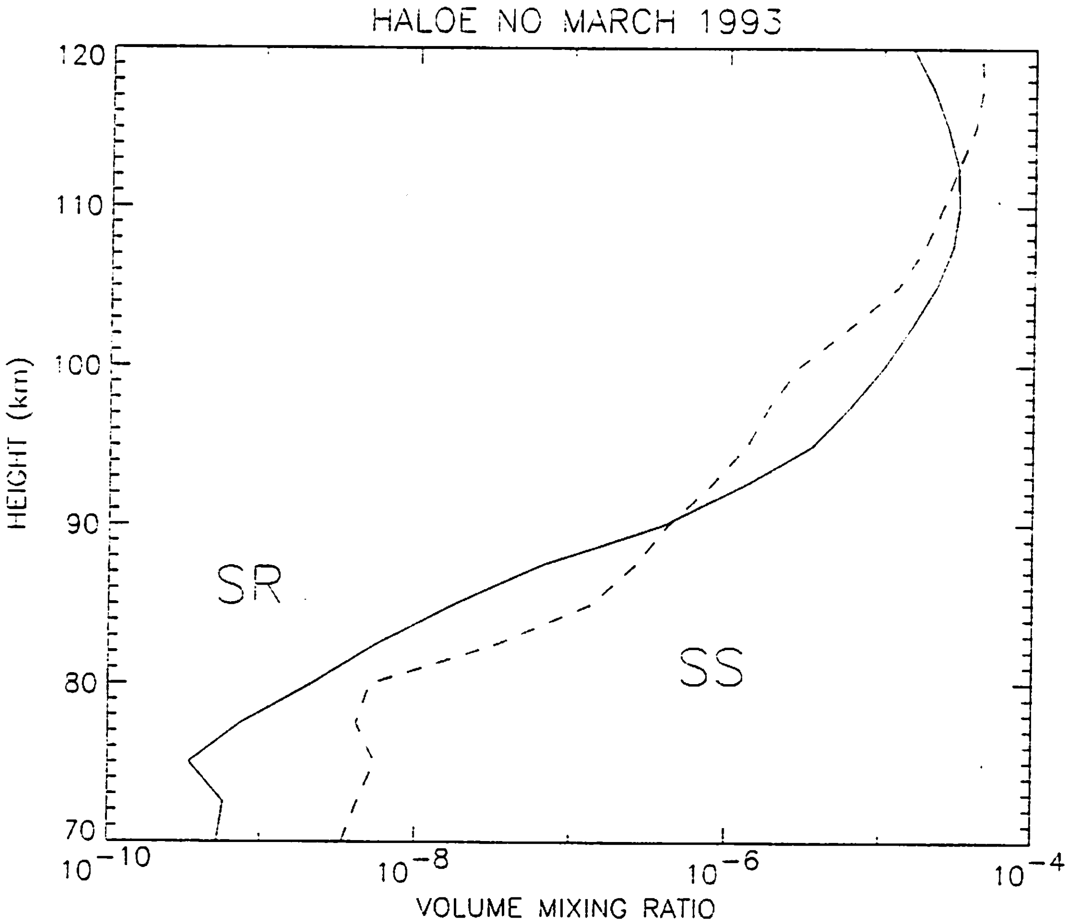
	τ	variability
gravity waves	hours	hours-seasonal
tides	hours	days-seasonal
planetary waves	days	weeks-seasonal
mean circulation	seasonal	annual

General rules:

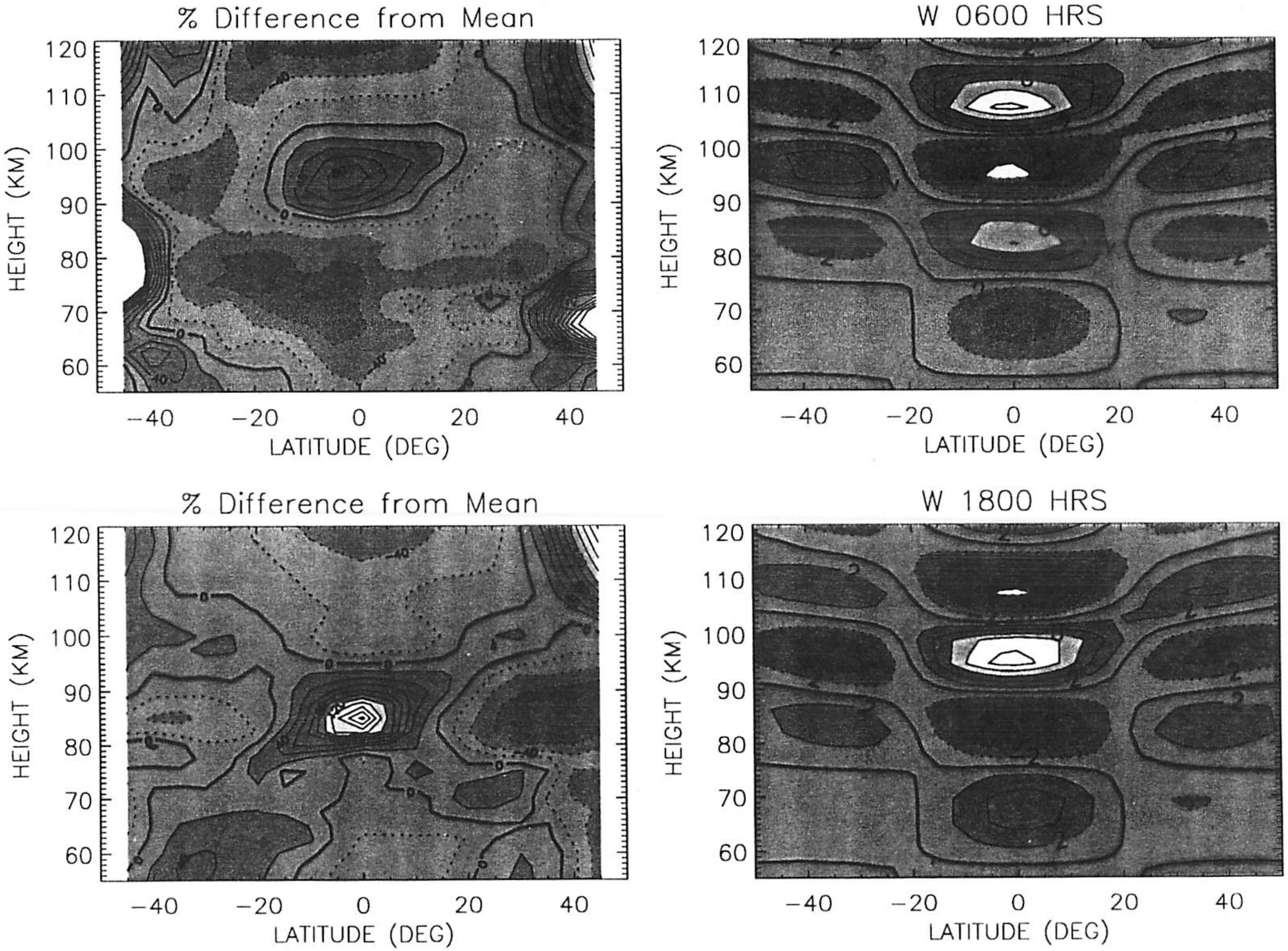
- time scale of variability increases with spatial scale

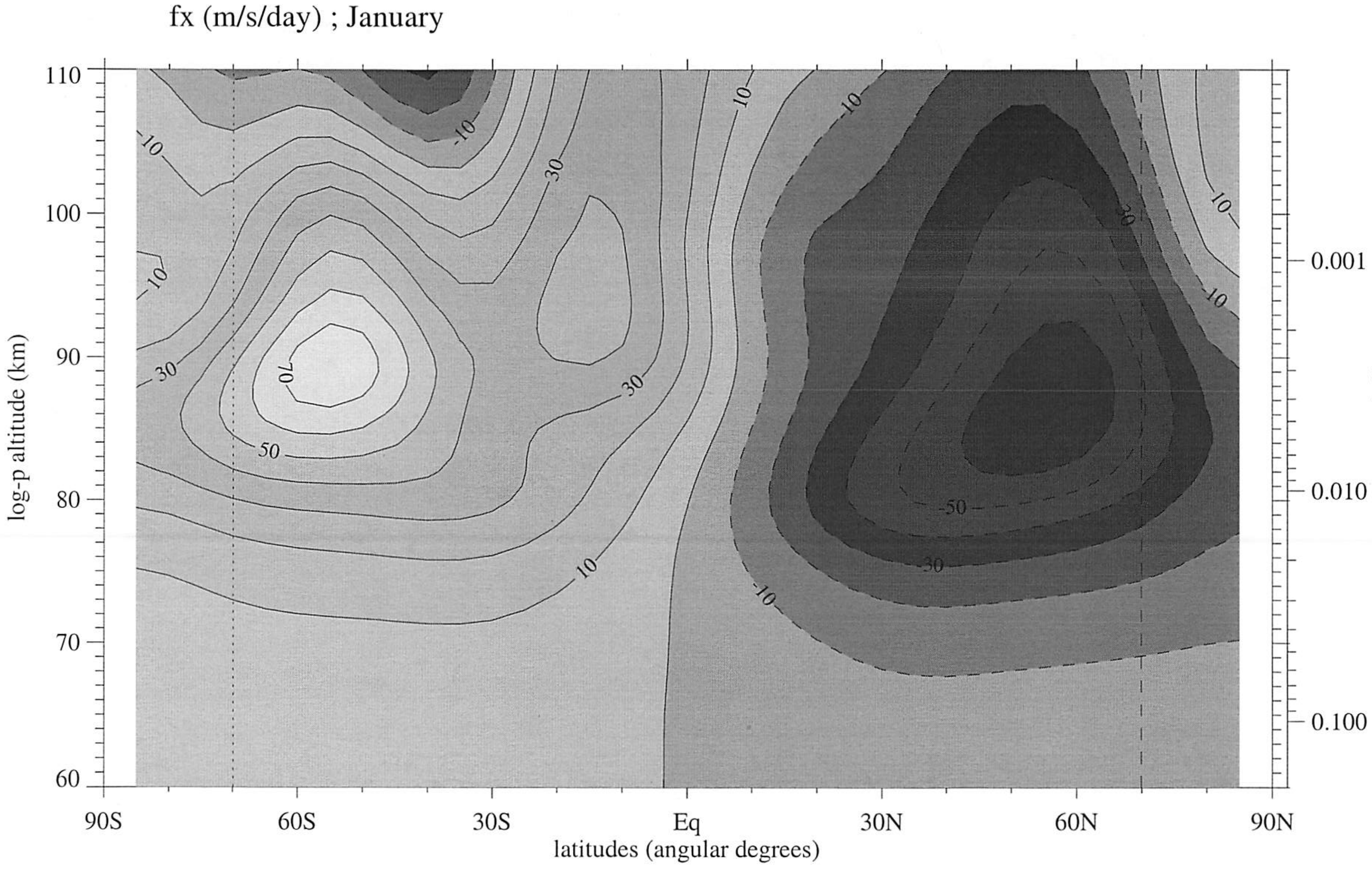
- propagation of low frequency waves (planetary and gravity waves) strongly affected by zonal wind

SUNRISE/SUNSET ANOMALY

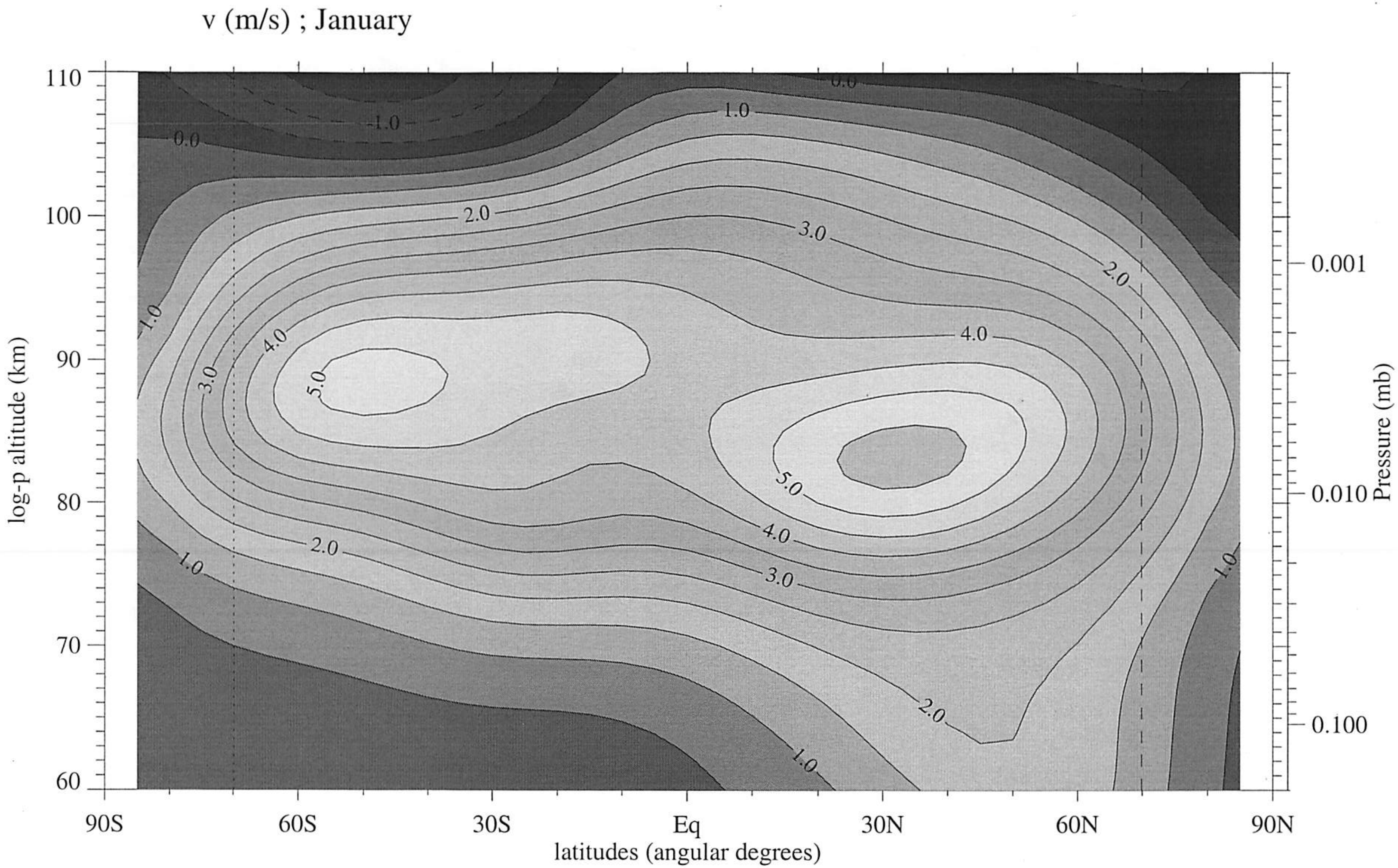


from Marsh & Russell, *GRL*, 2000

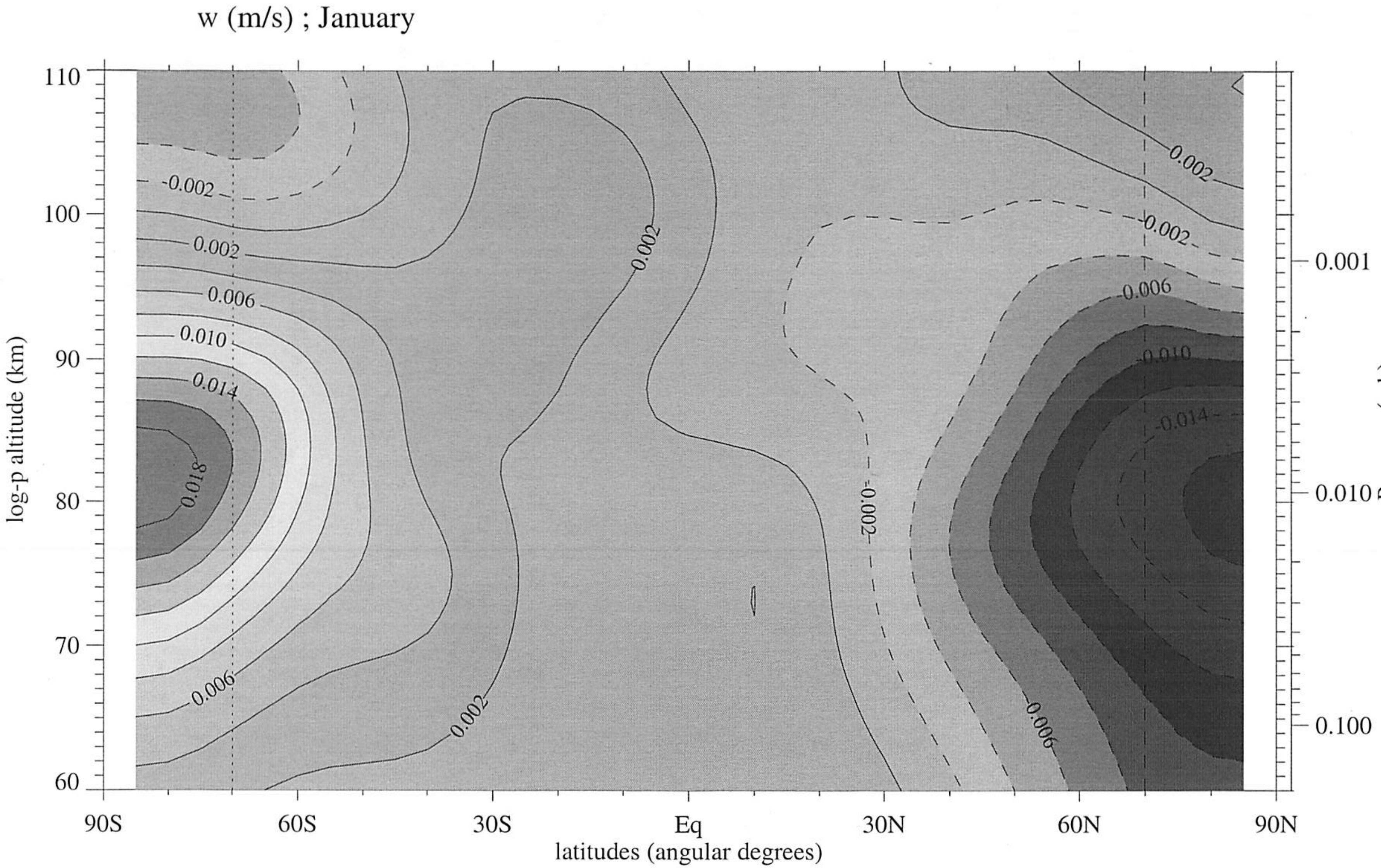

% Difference from Mean
W 0600 HRS
% Difference from Mean
W 1800 HRS
HEIGHT (KM)
LATITUDE (DEG)



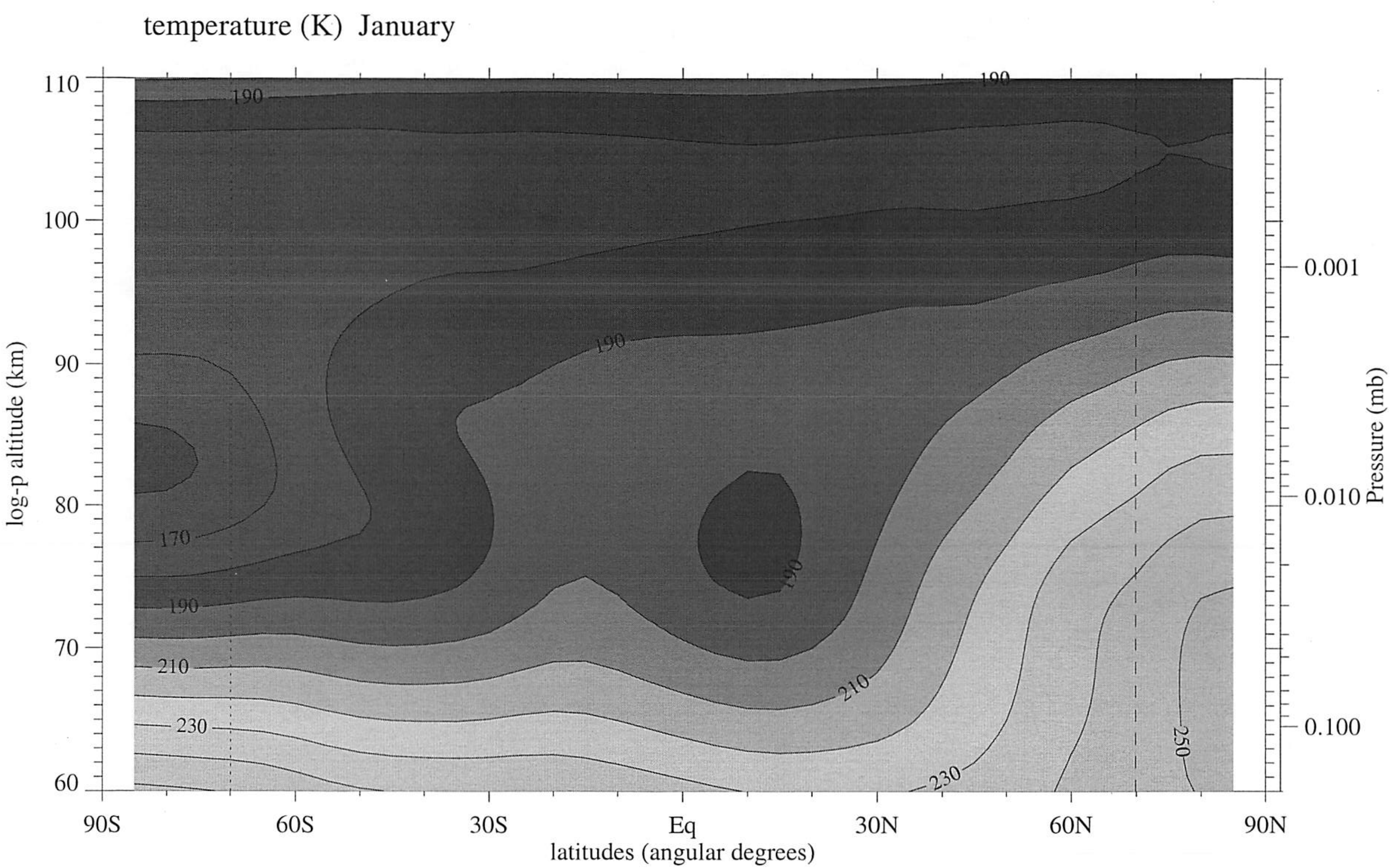
fx (m/s/day) ; January
log-p altitude (km)
110
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)
-10
10
30
50
70
-30
-50



v (m/s) ; January
log-p altitude (km)
110
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)
0.0
-1.0
1.0
2.0
3.0
4.0
5.0



w (m/s) ; January
110
100
90
80
70
60
log-p altitude (km)
-0.002
0.002
0.006
0.010
0.014
0.018
0.006
0.002
0.002
-0.002
0.002
-0.002
-0.006
-0.010
-0.014
-0.006
0.001
0.010
0.100
Pressure (mb)
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)


temperature (K) January
log-p altitude (km)
110
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)
190
190
190
170
190
210
230
210
230
250

Qualitative feature of the mean circulation

- momentum from wave dissipation drives summer to winter flow
- rising in summer, sinking in winter gives adiabatic forcing
- IR radiation responds to local temperature

but ....

- IR emissions are inefficient because of cold mesopause temperatures
- stronger temperature response than would occur for comparable momentum forcing in a warmer region

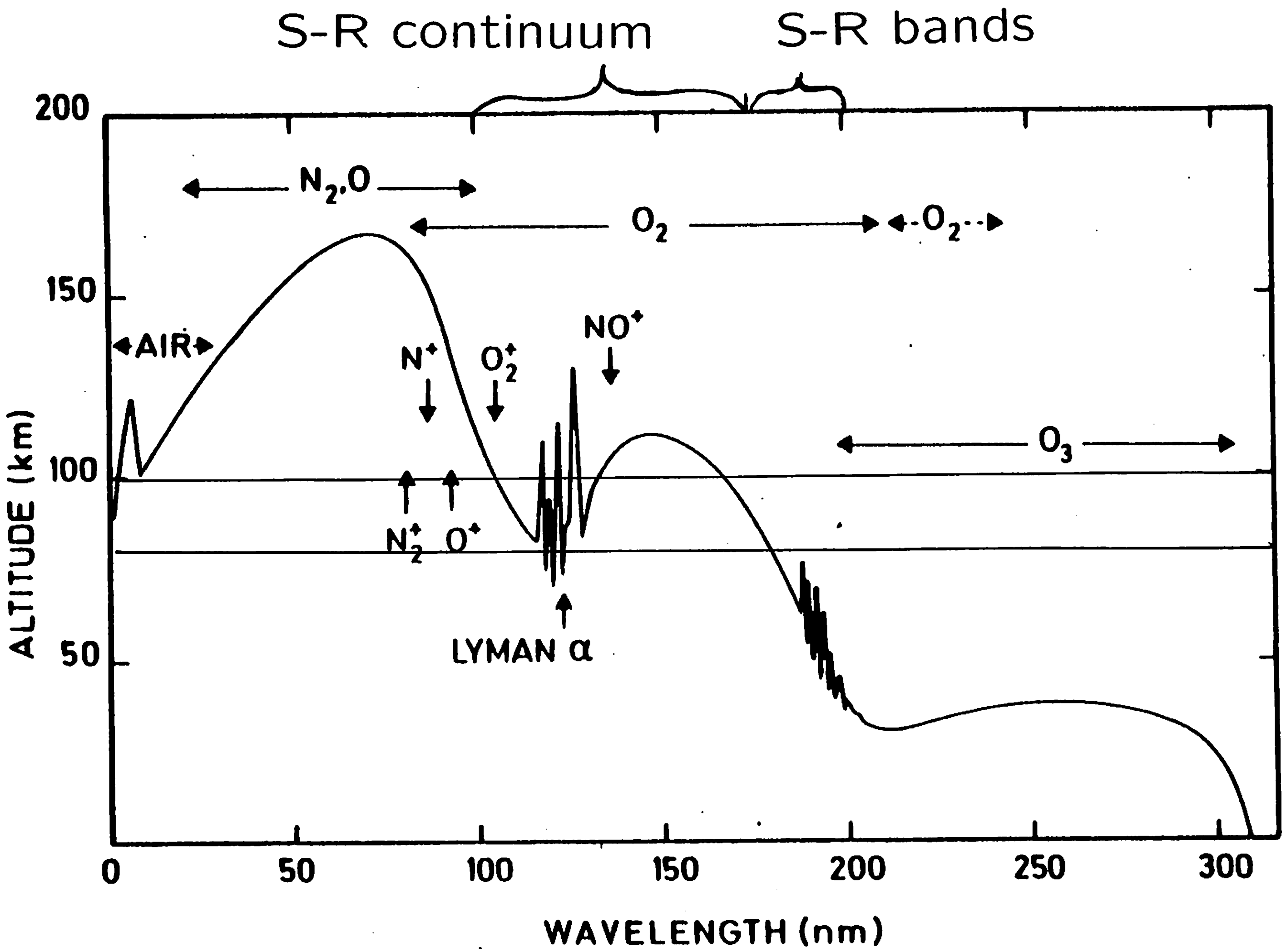
Impact of composition on energetics

absorption of solar radiation depends on composition:

- O_2: wavelengths 100-205 nm (Lyman-α, Schumann-Runge continuum, Schumann-Runge bands)
- O_3: wavelengths 242-310 nm (Hartley band)

absorbed energy goes into:

- breaking chemical bonds
- exciting vibrational or rotational levels of original absorber or its products
- converted immediately to heat



altitude at which flux is attenuated by 1/e

from Brasseur & Solomon, *Aeronomy of the Middle Atmosphere*

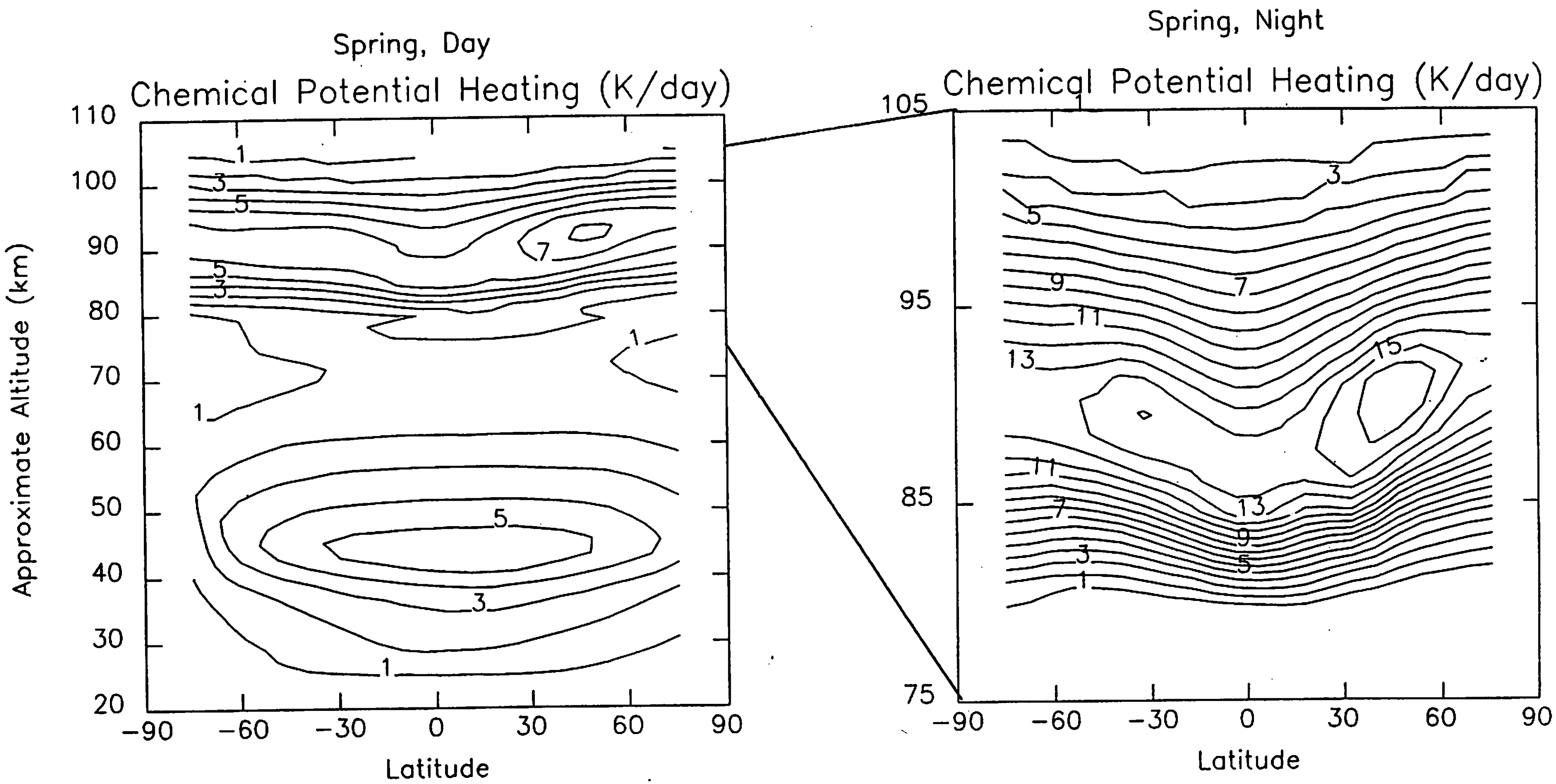
What happens to the energy of photolysis?

- energy used to break bonds is "stored" in the products and can be converted to heat when they react
- heat-releasing reactions can occur hours or days after and far away from original absorption

Reaction	
$O + O_3 \rightarrow O_2 + O_2$	
$O + O + M \rightarrow O_2 + M$	*
$O + OH \rightarrow H + O_2$	*
$O + HO_2 \rightarrow OH + O_2$	*
$H + O_2 + M \rightarrow HO_2 + M$	*
$O + O_2 + M \rightarrow O_3 + M$	*
$H + O_3 \rightarrow OH + O_2$	

* reaction rate decreases with temperature

Chemical Heating



from Mlynczak and Solomon, *JGR*, 1993

What happens to the energy of excited states?

converted to heat:

$$O_3 + h\nu \rightarrow O_2(^1\Delta_g) + O(^1D)$$

$$O_2(^1\Delta_g) + O_2 \rightarrow O_2 + O_2 + \text{heat}$$

transferred by collision:

$$O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g)$$

radiated out of region:

$$O_2(^1\Delta_g) \rightarrow O_2 + h\nu$$

$$O_2(^1\Sigma_g) \rightarrow O_2 + h\nu$$

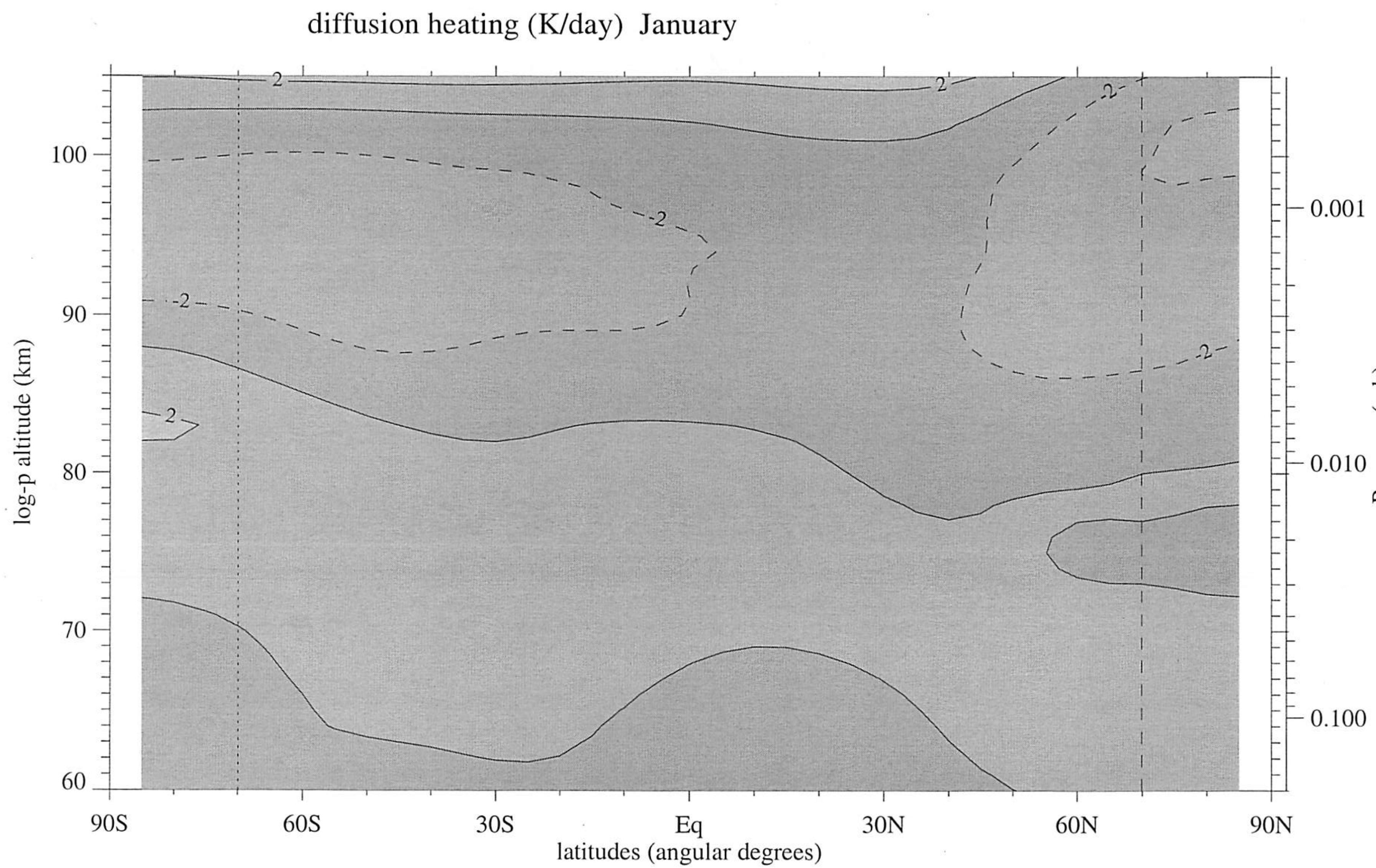
reacts:

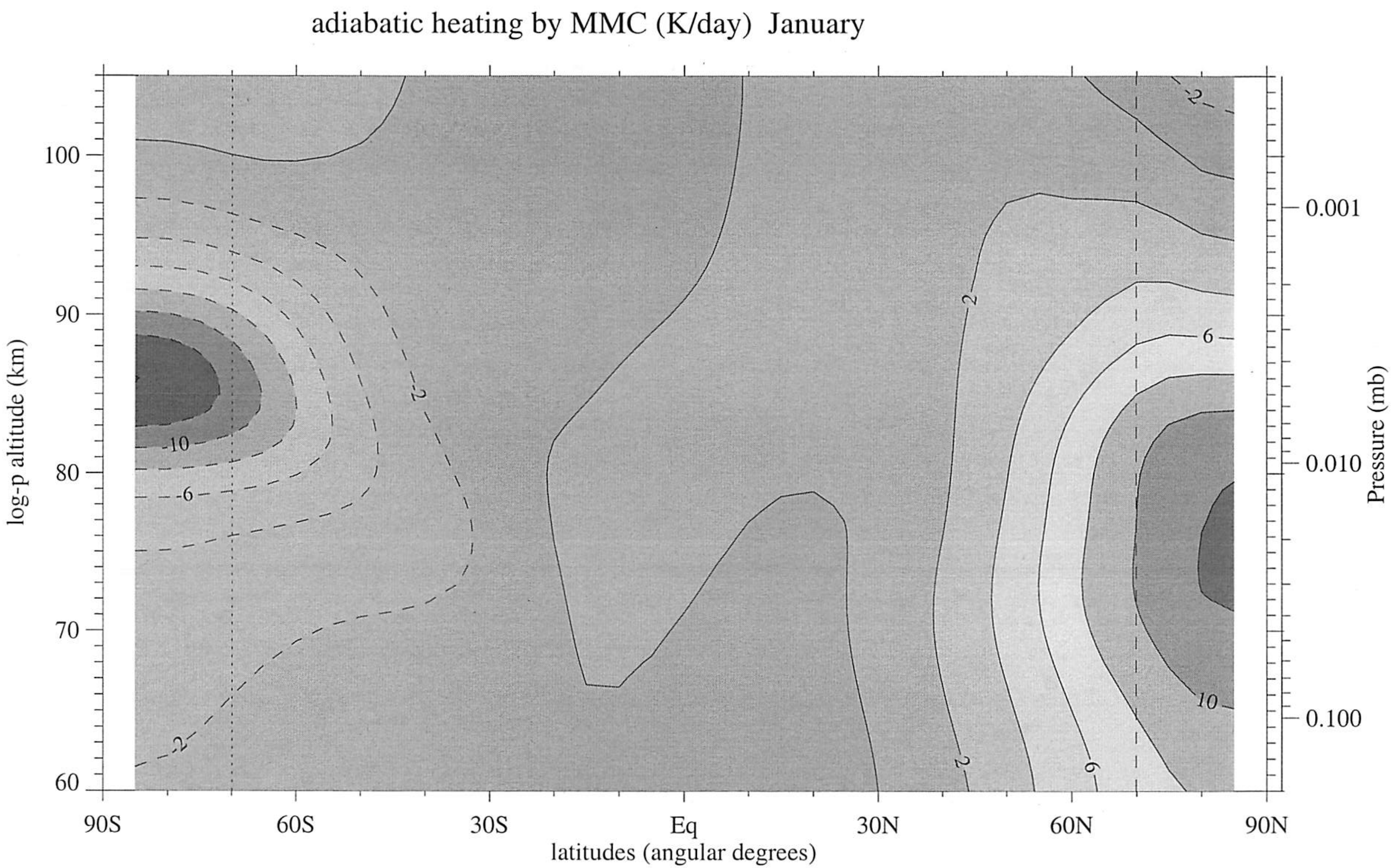
$$N(^2D) + O_2 \rightarrow NO + O$$

Magnitude & distribution of terms in the thermal budget

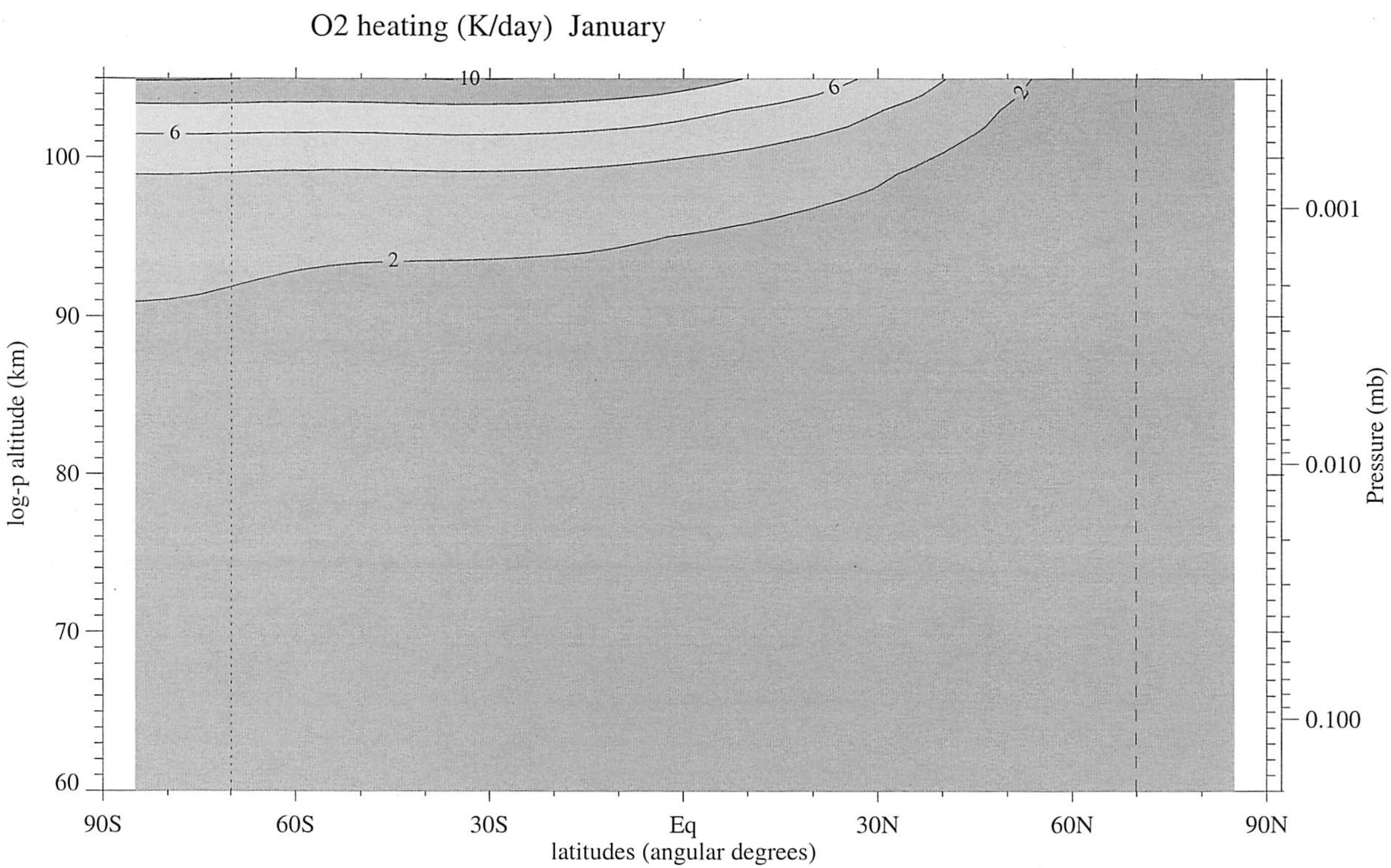
- diffusion
- advection by the mean circulation
- direct solar O_2 heating*
- direct solar O_3 heating*
- chemical heating*
- infrared cooling

* minus fraction lost through emission (airglow)


diffusion heating (K/day) January
log-p altitude (km)
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
2
-2
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)

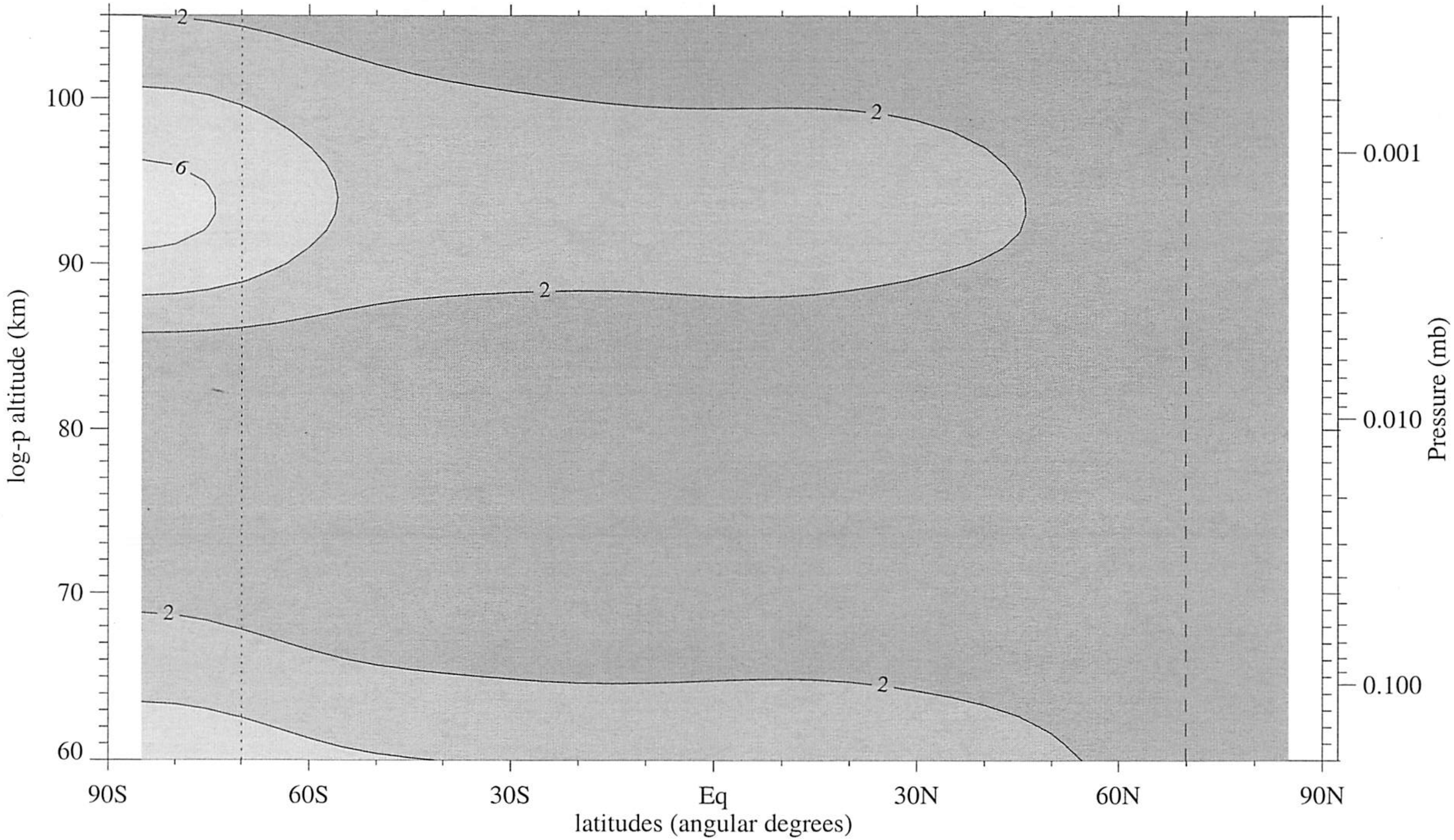


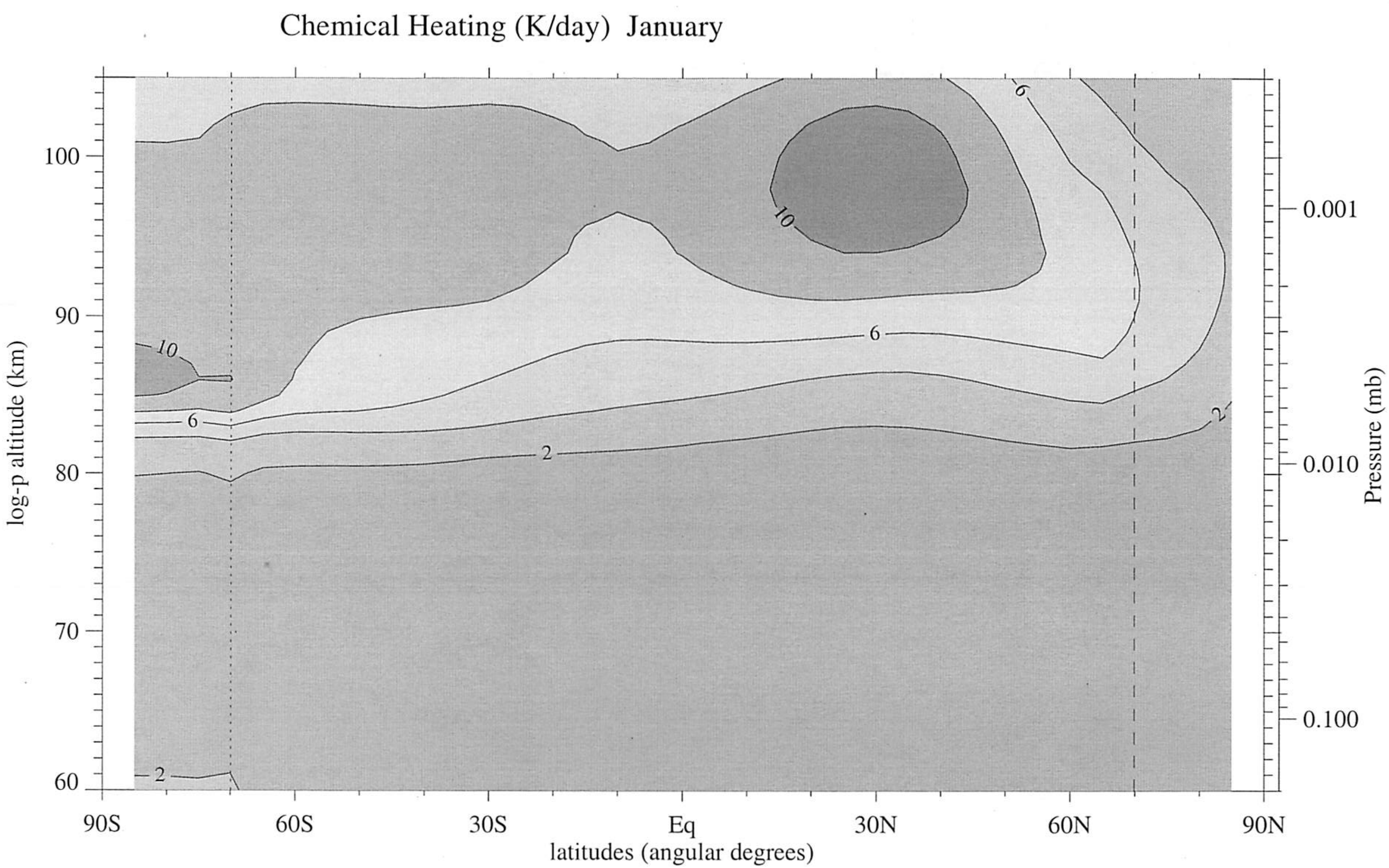
adiabatic heating by MMC (K/day) January
log-p altitude (km)
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)
-2
-6
-10
2
6
10



O2 heating (K/day) January
10
6
6
2
6
2
100
90
80
70
60
log-p altitude (km)
0.001
0.010
0.100
Pressure (mb)
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)

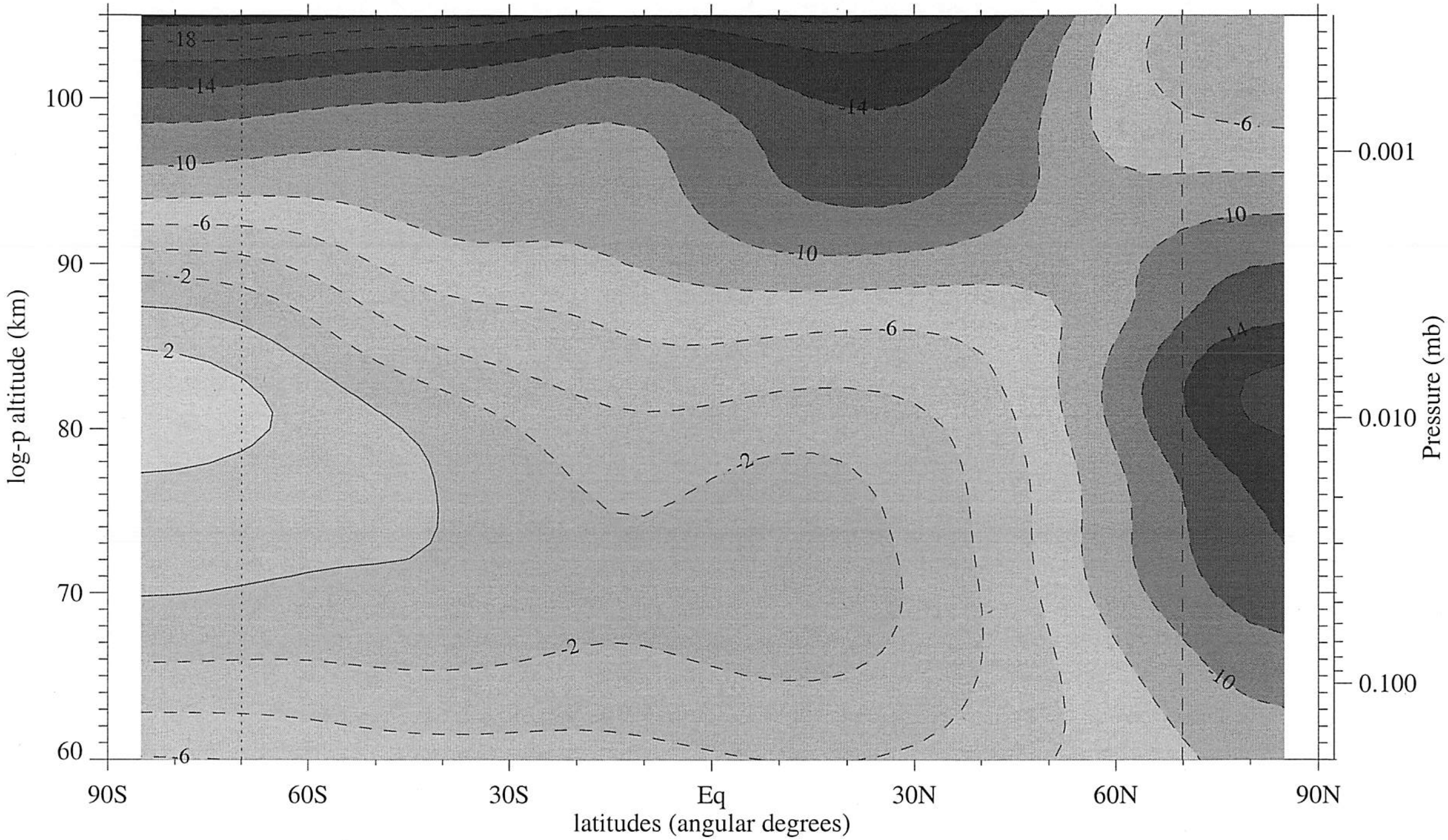
O3 heating (K/day) January





Chemical Heating (K/day) January
log-p altitude (km)
100
90
80
70
60
Pressure (mb)
0.001
0.010
0.100
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)
10
6
2

radiative cooling (K/day) January



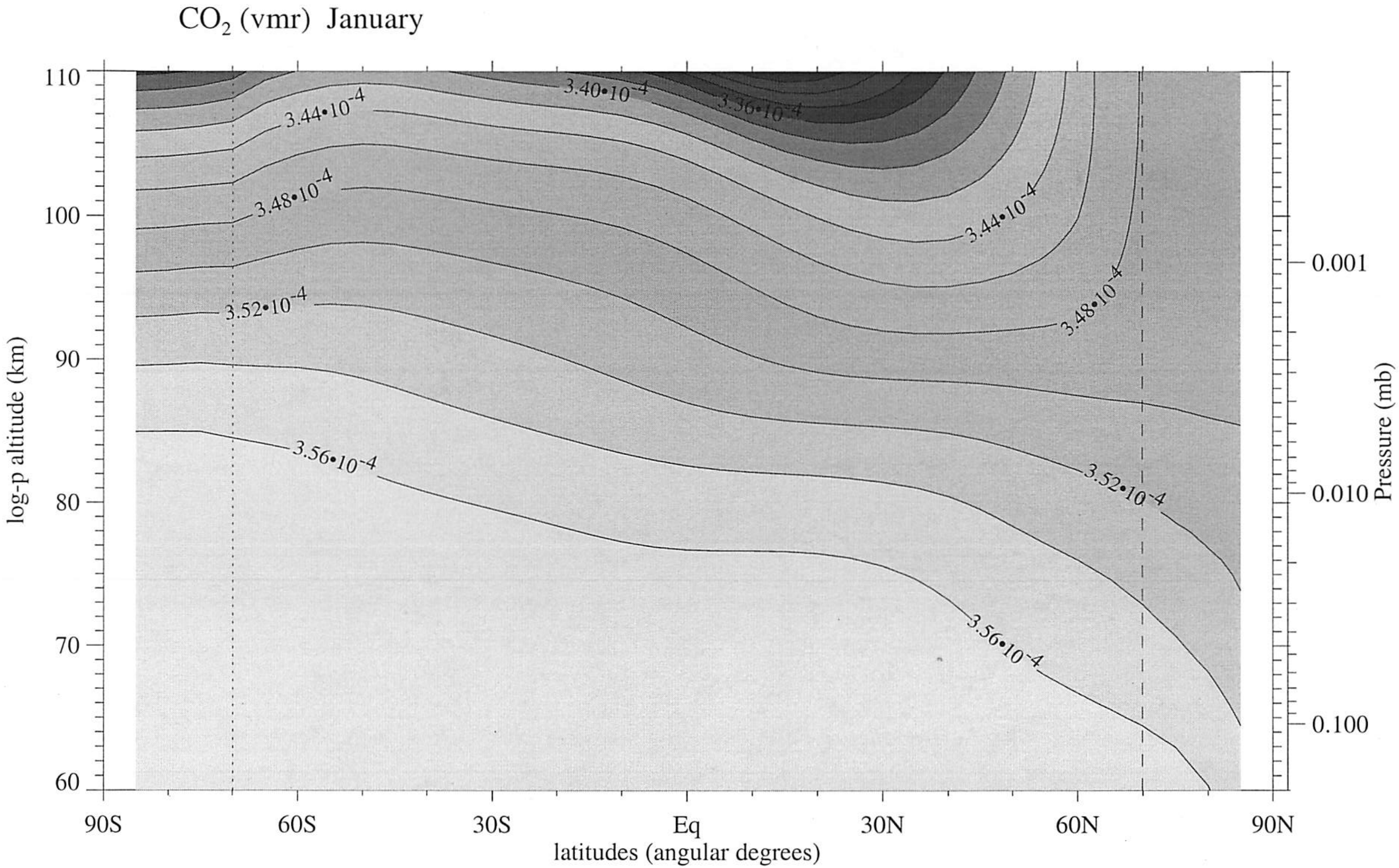
EXAMPLE OF INTERACTION

polar mesopause temperature determined by:

- adiabatic processes of wave-driven circulation
- heating & cooling (CO_2 cooling rate; chemical heating)

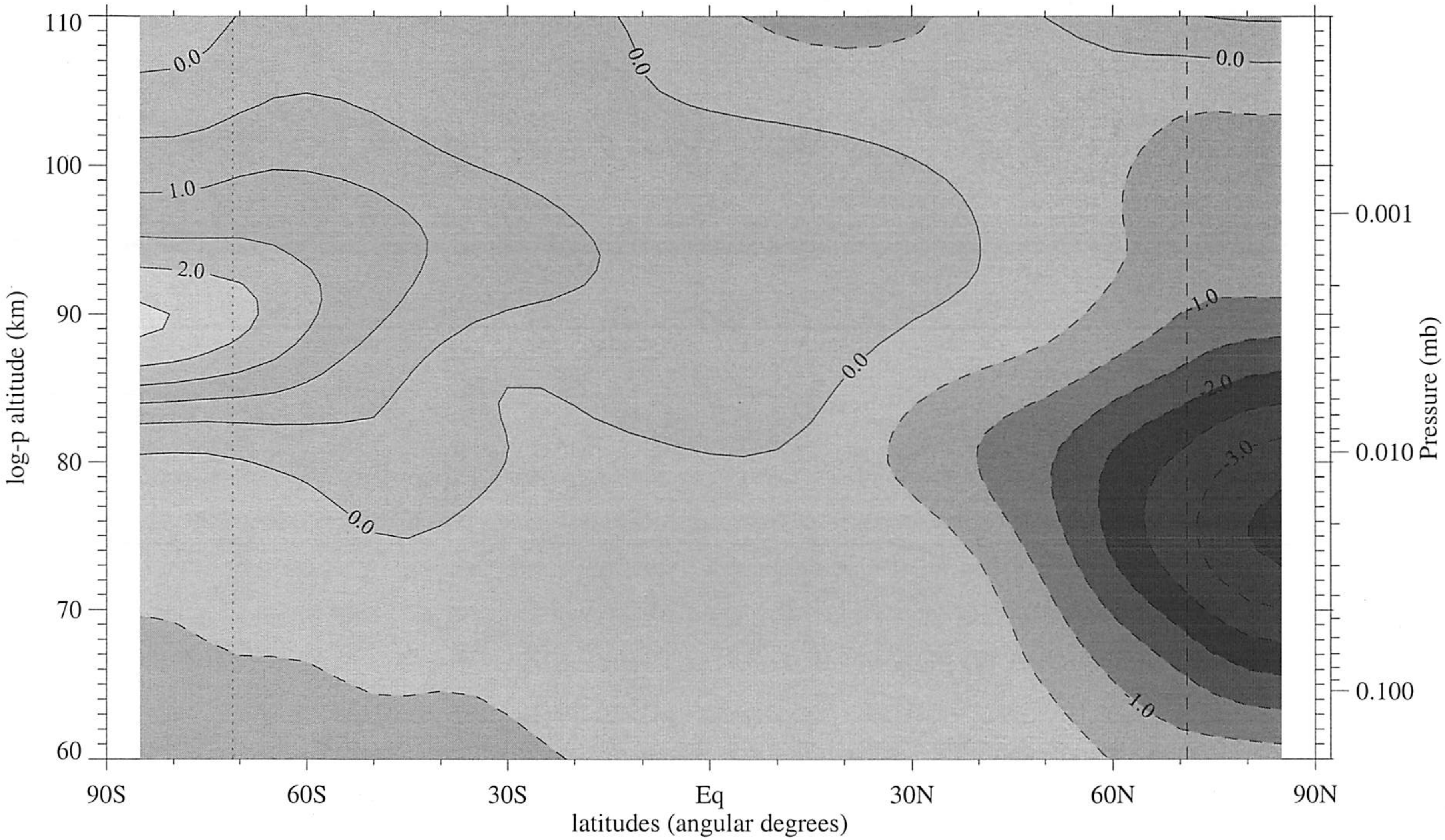
upward motion (summer pole):

- adiabatic cooling
- high CO_2
- enhancement to IR cooling



CO2 (vmr) January
110
100
90
80
70
60
log-p altitude (km)
3.40•10-4
3.36•10-4
3.44•10-4
3.48•10-4
3.52•10-4
3.56•10-4
0.001
0.010
0.100
Pressure (mb)
90S
60S
30S
Eq
30N
60N
90N
latitudes (angular degrees)

temperature difference (K) due to uniform CO2 January

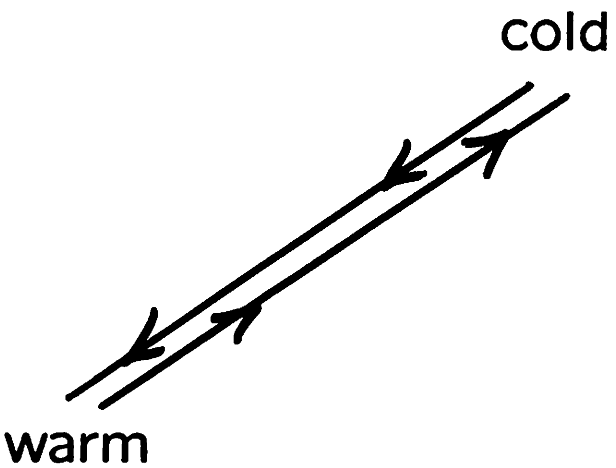


IMPACT OF GLOBAL CO_2 STRUCTURE

- positive feedback
- enhances the cold summer, warm winter temperature differences
- model results may underestimate magnitude because of neglect of molecular diffusion

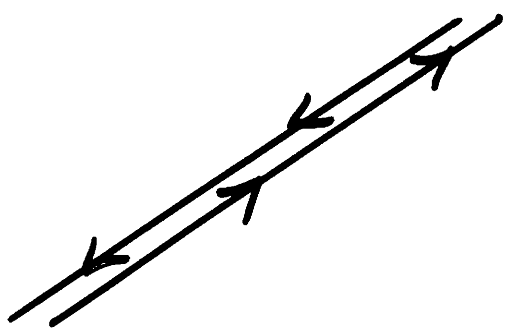
Photochemical Destabilization of gravity waves

Air parcel trajectory in a propagating gravity wave



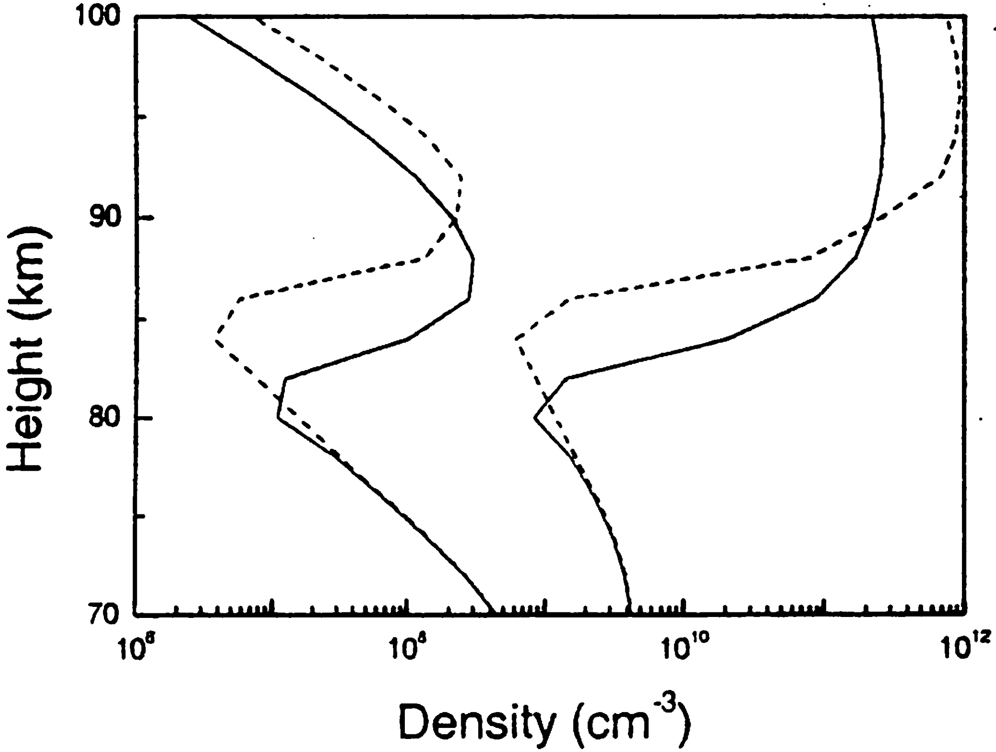
Composition and density

high O, total density low

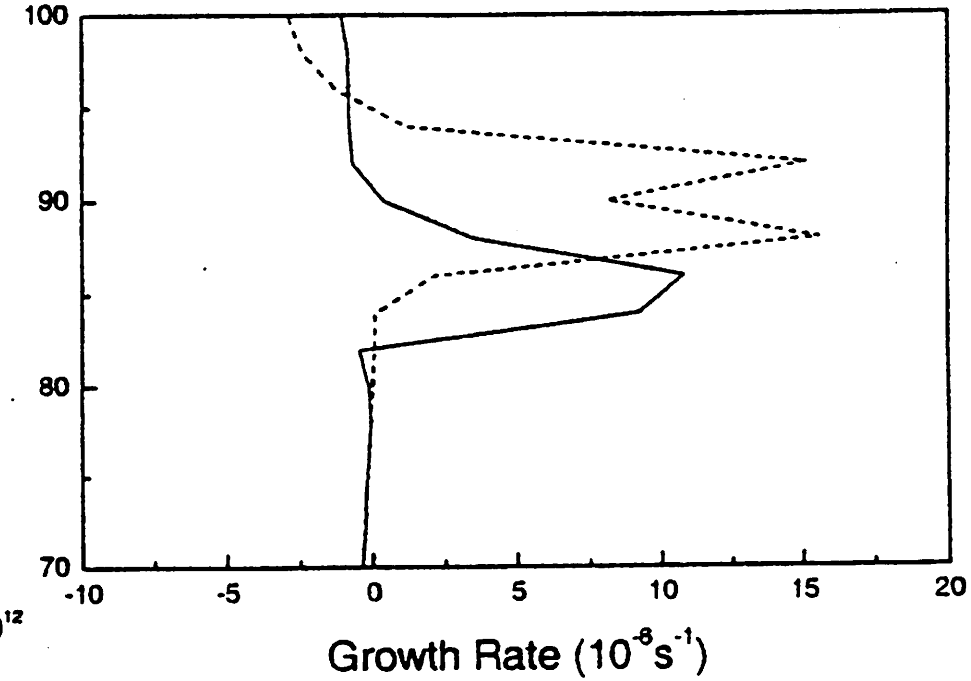


lower O, higher total density

midnight density of O and O_3



gravity wave unstable growth rate

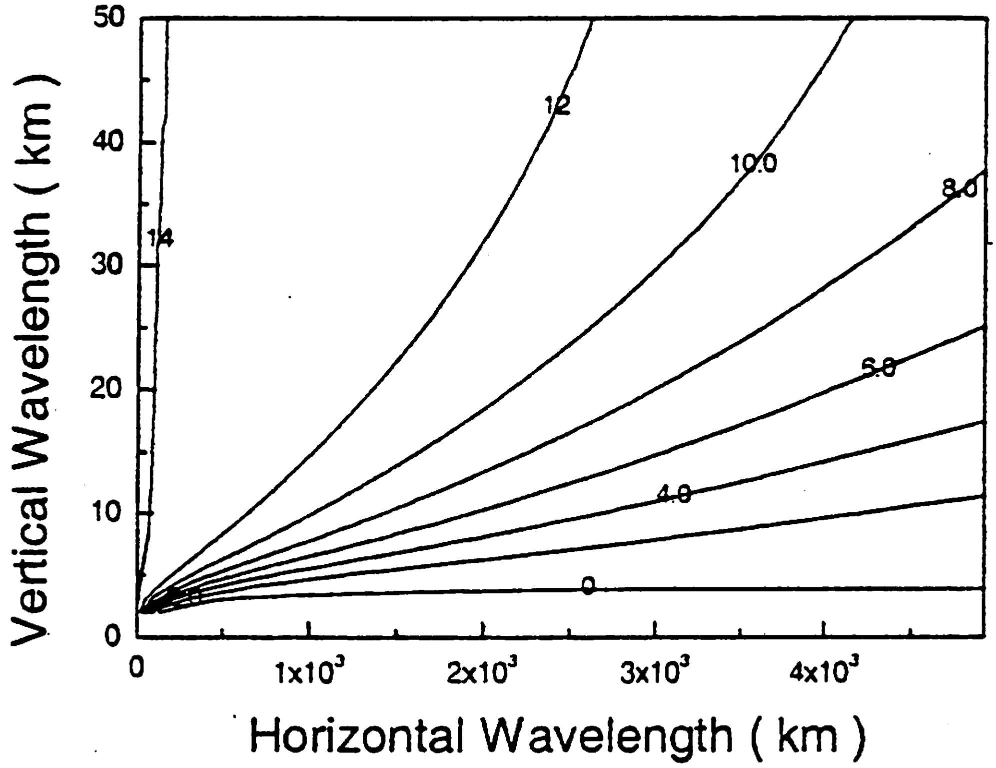


solid: K_{zz} high; w=0

dashed: K_{zz} low; w=upward

from Xu et al. *JASTP*, in press

variation in growth rate with wavelength



cutoff for $K_{zz} = 10^2 m^2/s$

Photochemical destabilization more likely for:

- low temperature
- low diffusion
- sharp vertical gradients of O
- long vertical, short horizontal wavelengths

Composition

- variability
  - regular diurnal, seasonal and interannual time scales
  - irregular variability due to forcing from above (energy) and below (waves)
- feedback
  - affects all scales of motion from mean circulation to individual gravity waves
  - controls the conversion of energy to heat