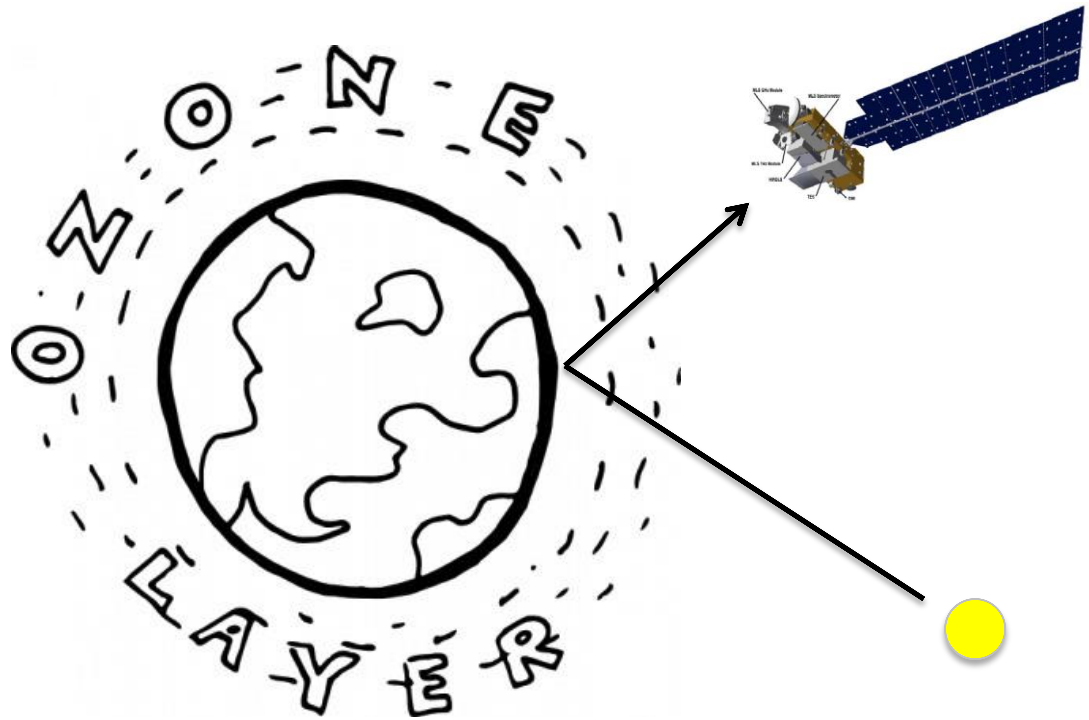


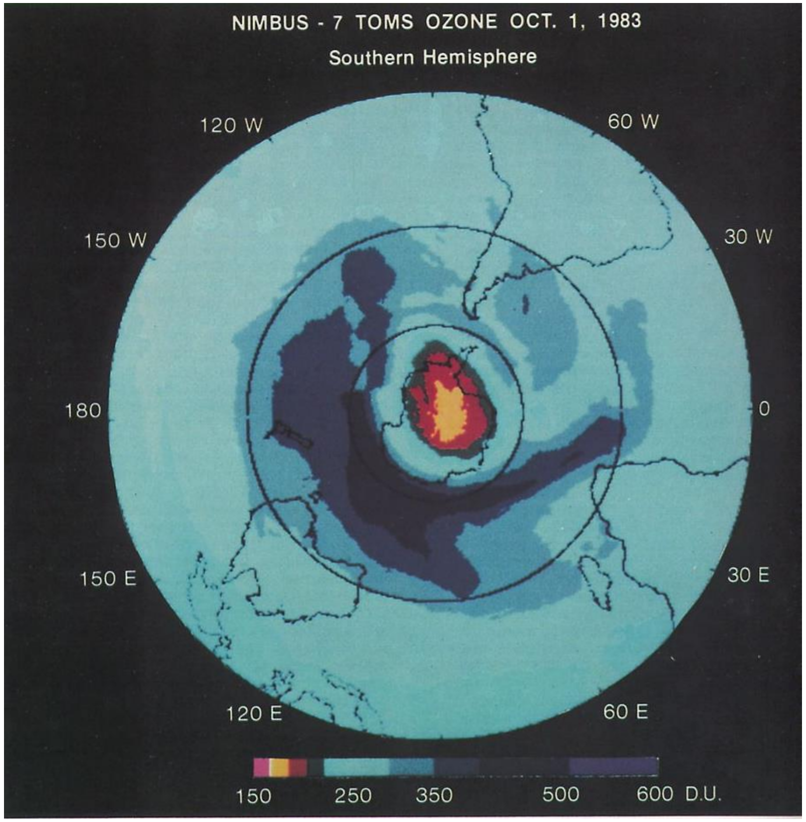
V9 total ozone and profile algorithm

11:00 – 11:50 Lectures III

David Haffner (SSAI, NASA/GSFC) and
P.K. Bhartia (GSFC, NASA)

TOMS-Derived Images of Antarctic Ozone Hole

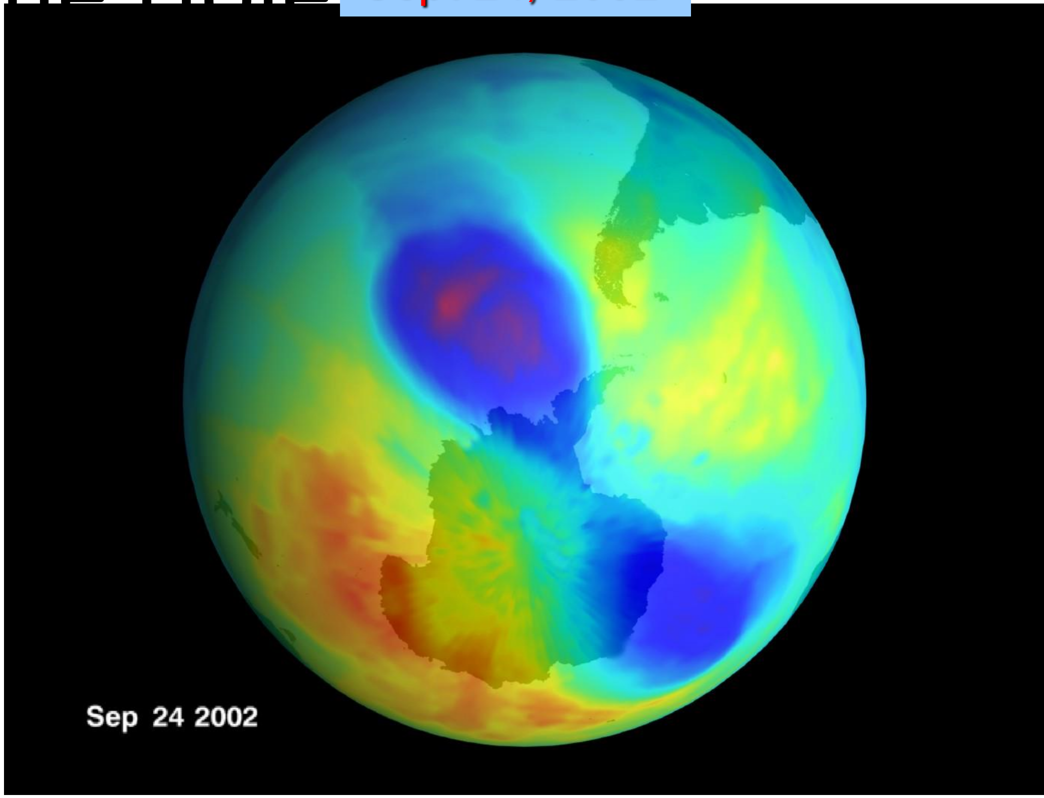
Oct 1, 1983



1st Image
Nimbus-7 TOMS

Bhartia et al., ‘85

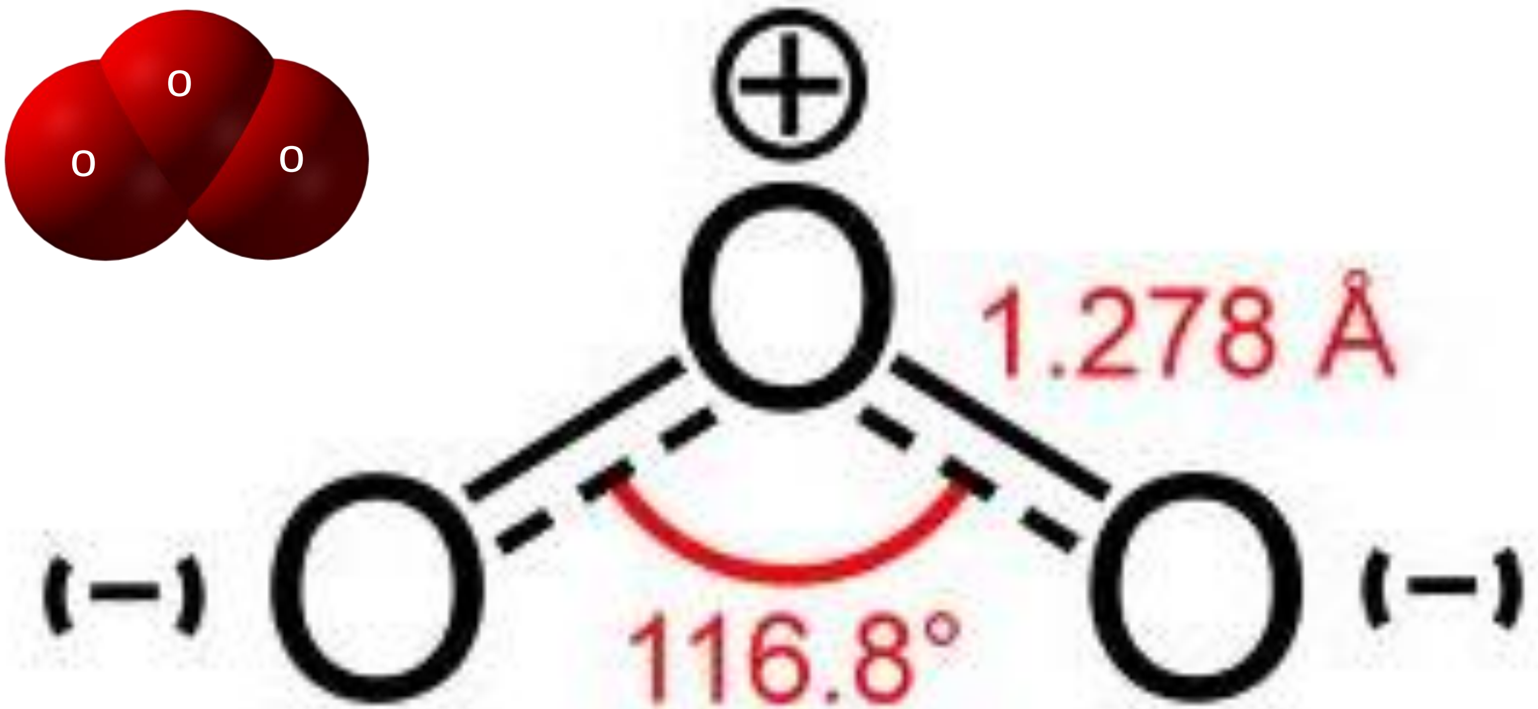
Sept 24, 2002

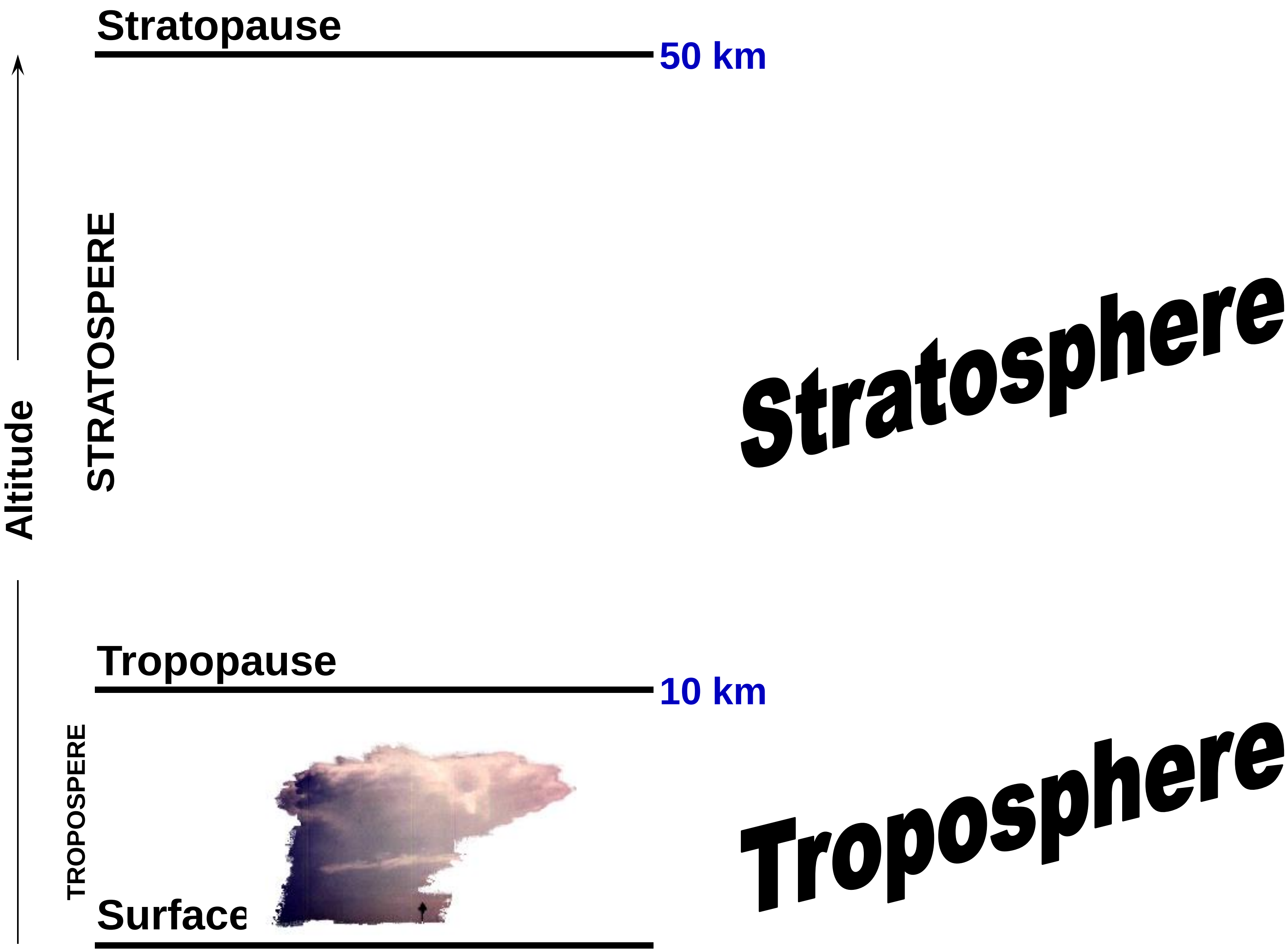


Modern Image
EP/TOMS

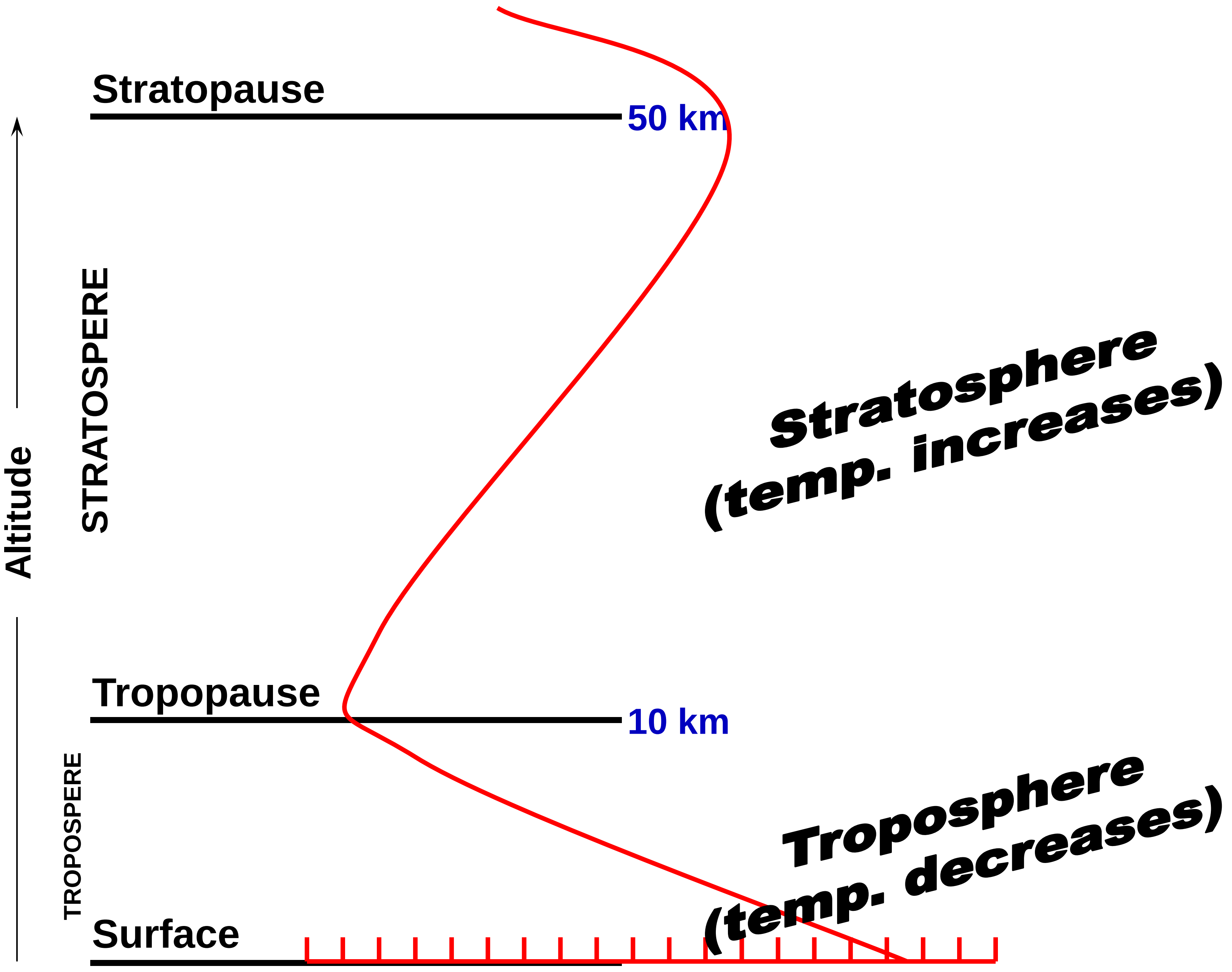
ozonewatch.gsfc.nasa.gov

A Brief Introduction to Atmospheric Ozone (O_3)

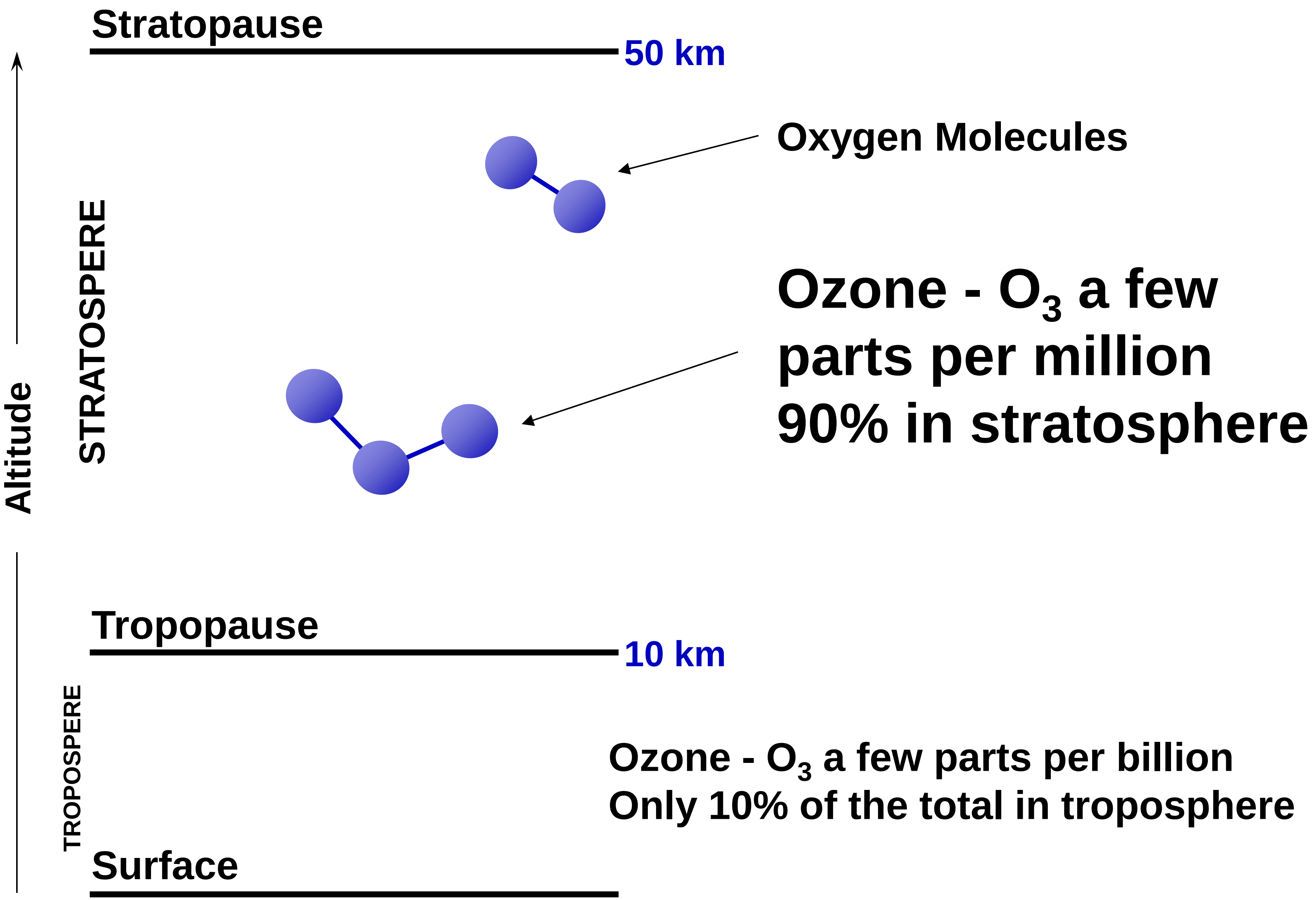




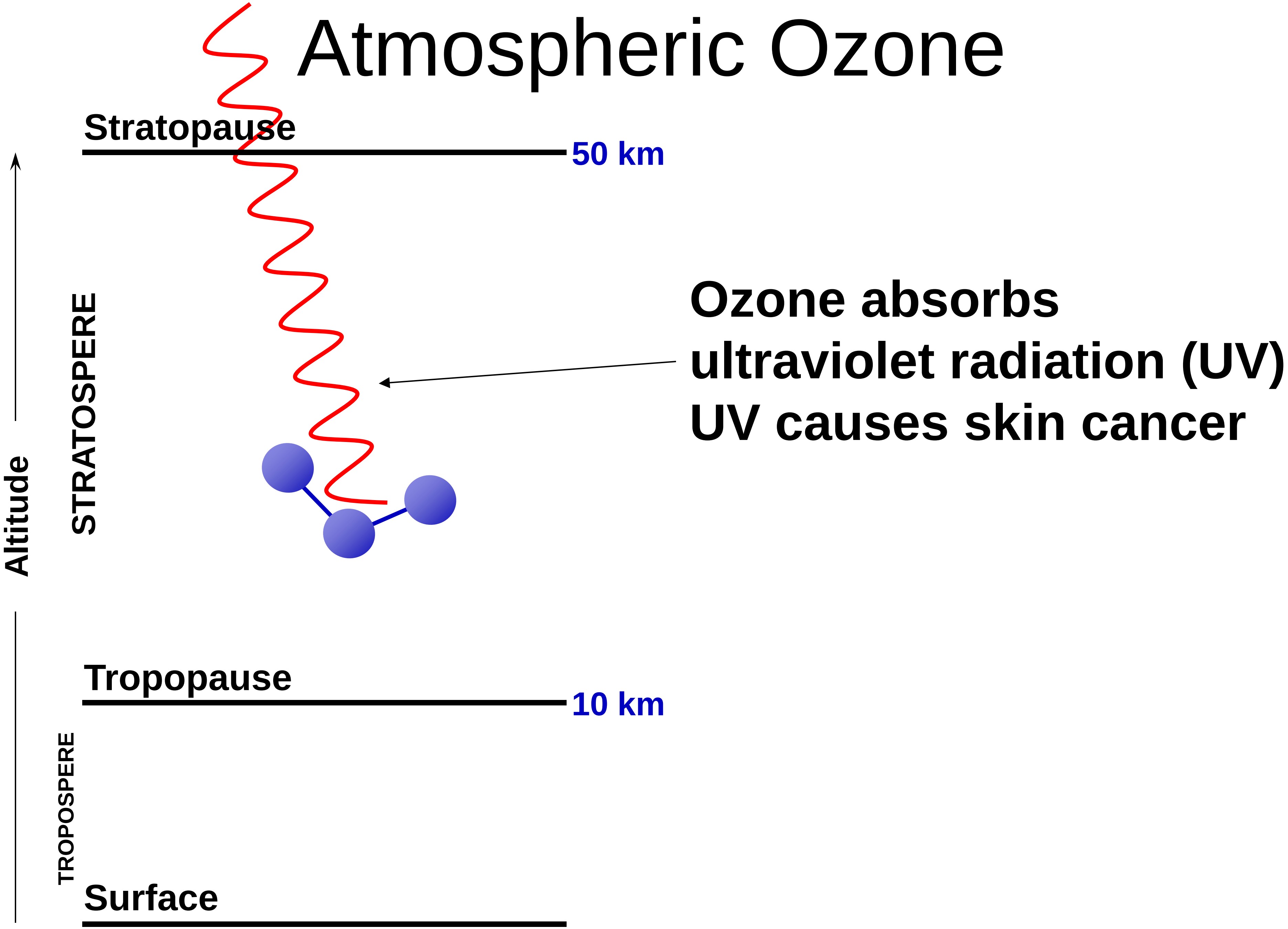
Stratopause
50 km
Altitude
STRATOSPERE
Stratosphere
Tropopause
10 km
TROPOSPERE
Troposphere
Surface


Stratopause
50 km
Altitude
STRATOSPERE
Stratosphere
(temp. increases)
Tropopause
10 km
TROPOSPERE
Troposphere
(temp. decreases)
Surface
Temperature (K)

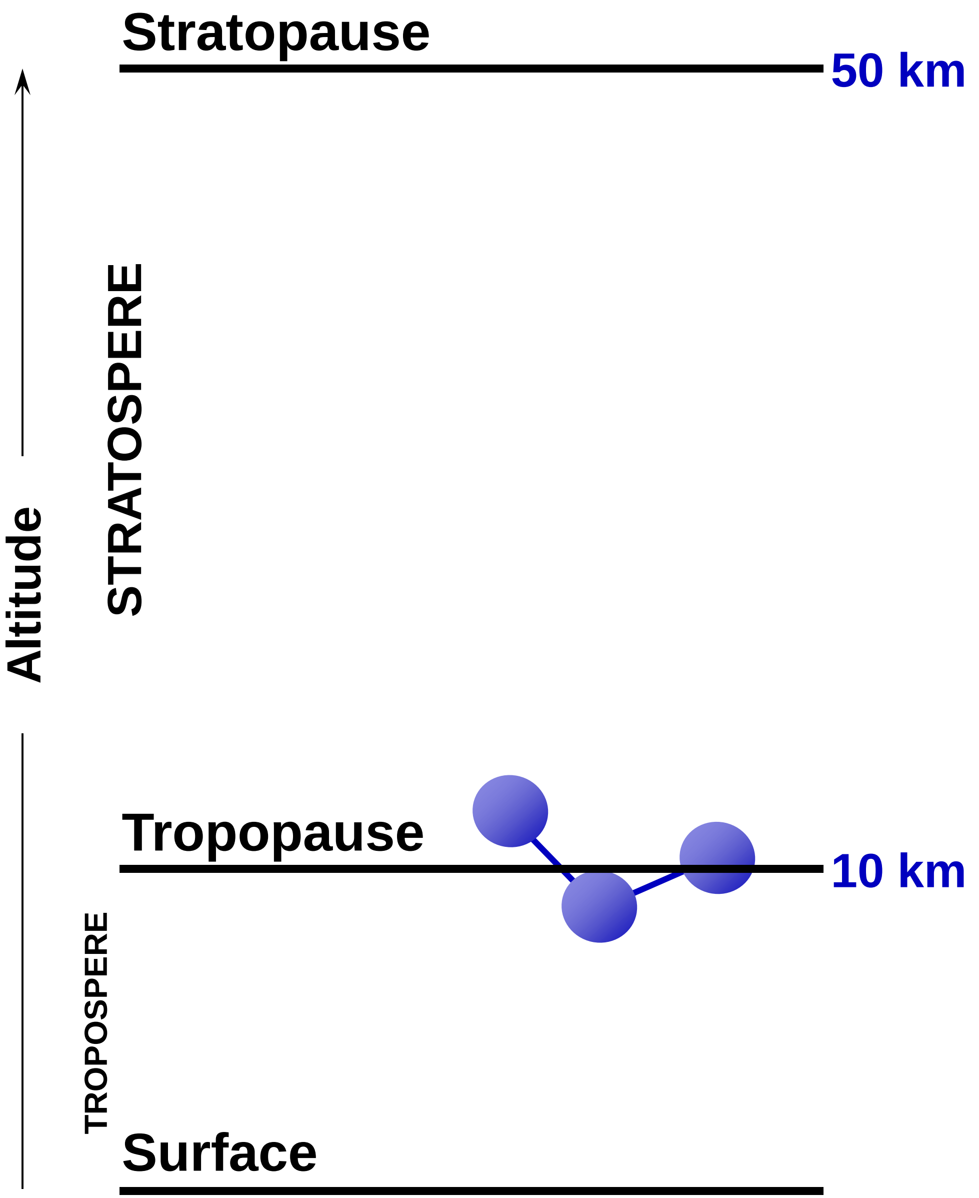
Atmospheric Ozone



Atmospheric Ozone

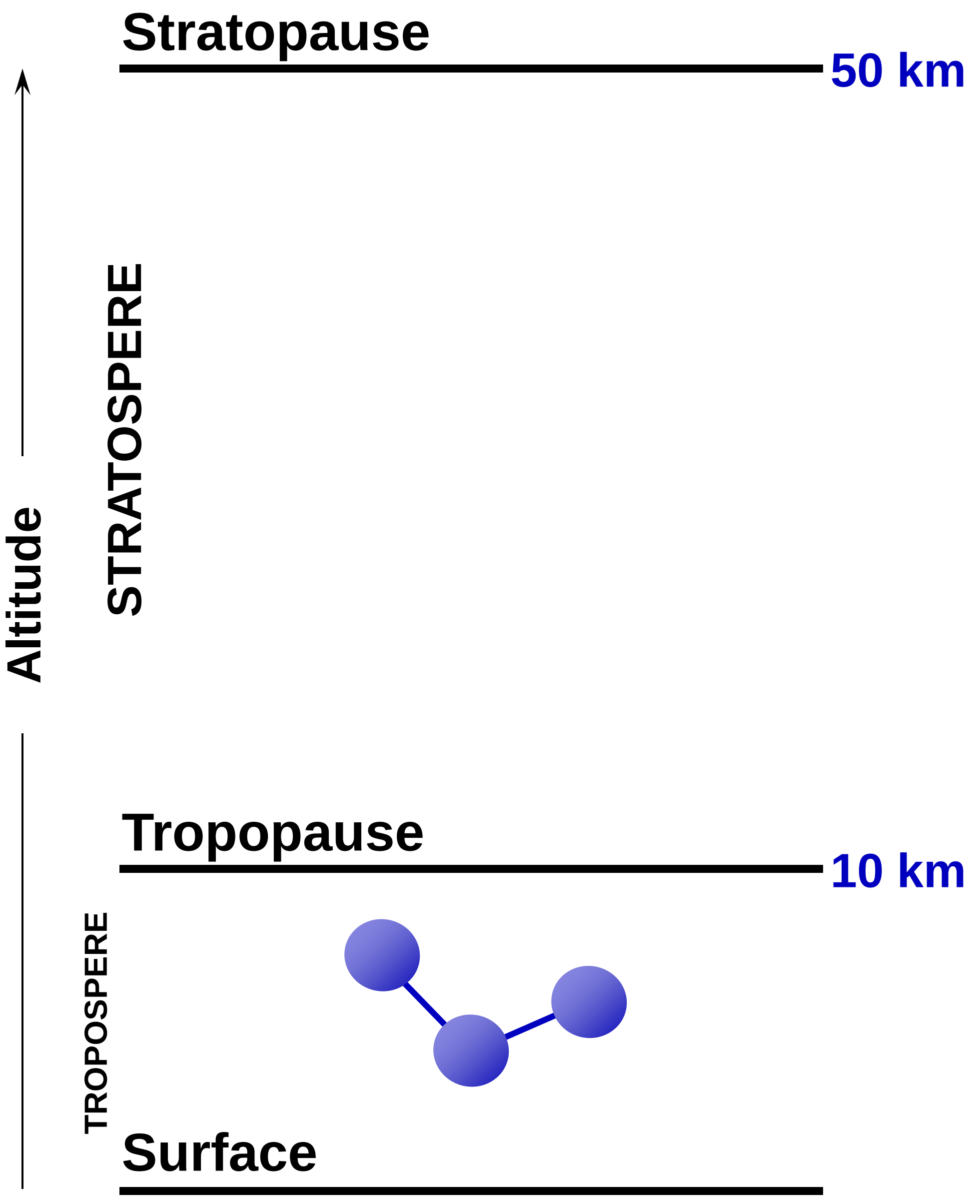


Atmospheric Ozone



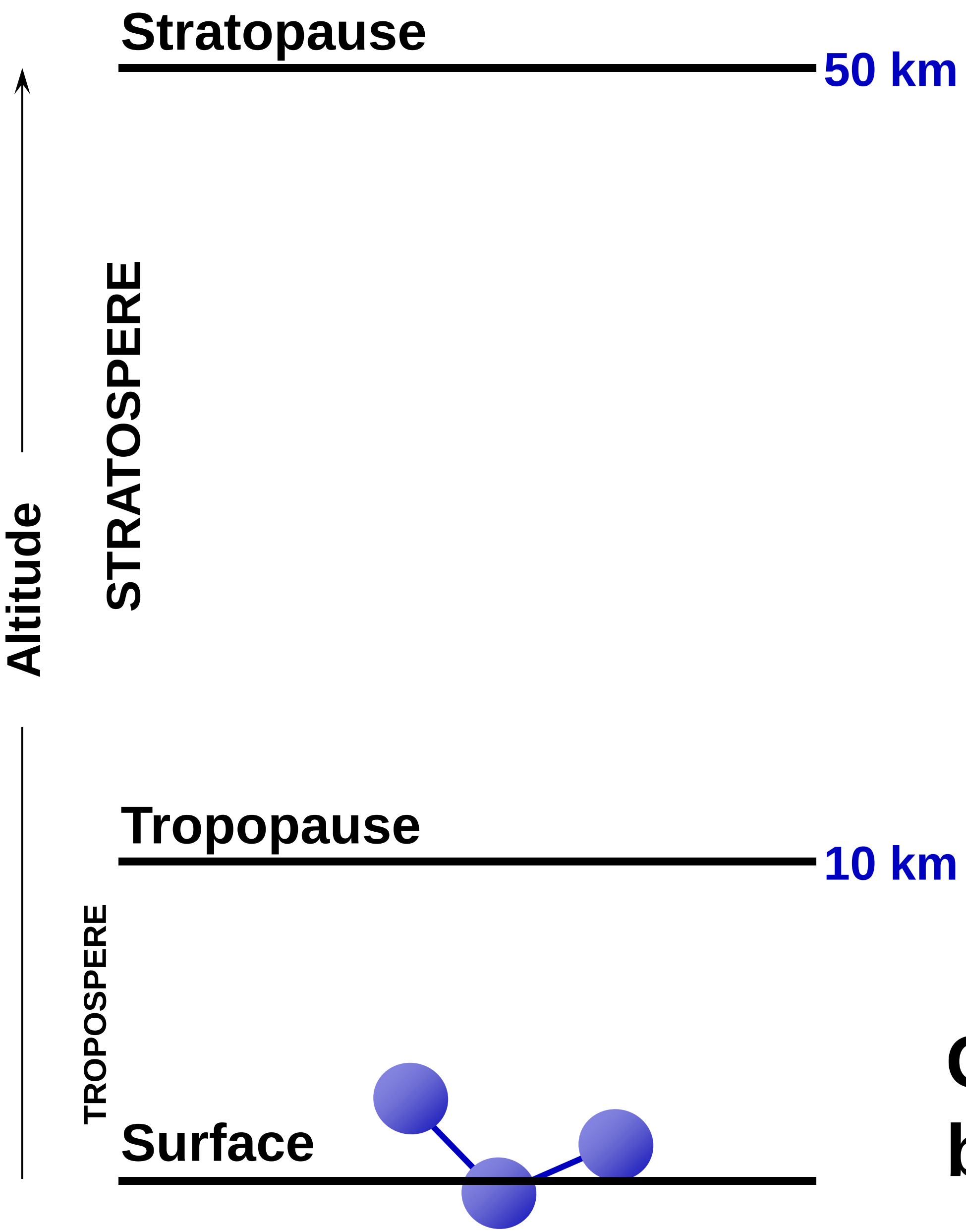
Ozone is a greenhouse gas

Atmospheric Ozone



Ozone produces OH radical which cleans the atmosphere of pollutants

Atmospheric Ozone



Ozone itself becomes a pollutant

Total O_3 Accuracy and Precision from the TOMS Algorithm

JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 89, NO. D4, PAGES 5239–5247, JUNE 30, 1984

Intercomparison of the NIMBUS 7 SBUV/TOMS Total Ozone Data Sets With Dobson and M83 Results

P. K. Bhartia, K. F. Klenk, C. K. Wong, and D. Gordon

Systems and Applied Sciences Corporation

A. J. Fleig

Laboratory for Atmospheric Sciences, NASA Goddard Space Flight Center

Key Conclusion

……TOMS instrument is producing daily global ozone maps with between 50 and 150 km resolution; each measurement on this map has accuracy and precision comparable to the best-run stations in the Dobson network.

Motivations for GEO Total Ozone Measurement

– *Model evaluation*

Improved knowledge of Tropospheric O_3 and Radiative forcing when combined with MLS O_3 and OMI OCP data (Joiner et al., 2009).

– *Data assimilation: O_3 knowledge improves analyses of lower stratosphere dynamics*

- Operational NWP: NCEP, ECMWF
- Regional (E. Asian!) dust and chemical weather models
- Chemistry & climate models: GEOS-CHEM, GEOS-5, MERRA
- Total column provides important model constraint

– *Dynamical studies*

Tracer for short-term variability and dynamical events in lower stratosphere.

Motivations for GEO Total Ozone Measurement

- *Tropospheric studies*

  O_3 mixing ratios in Deep Convective Clouds, independent of stratospheric information (Ziemke, 2009) and classic residual methods.

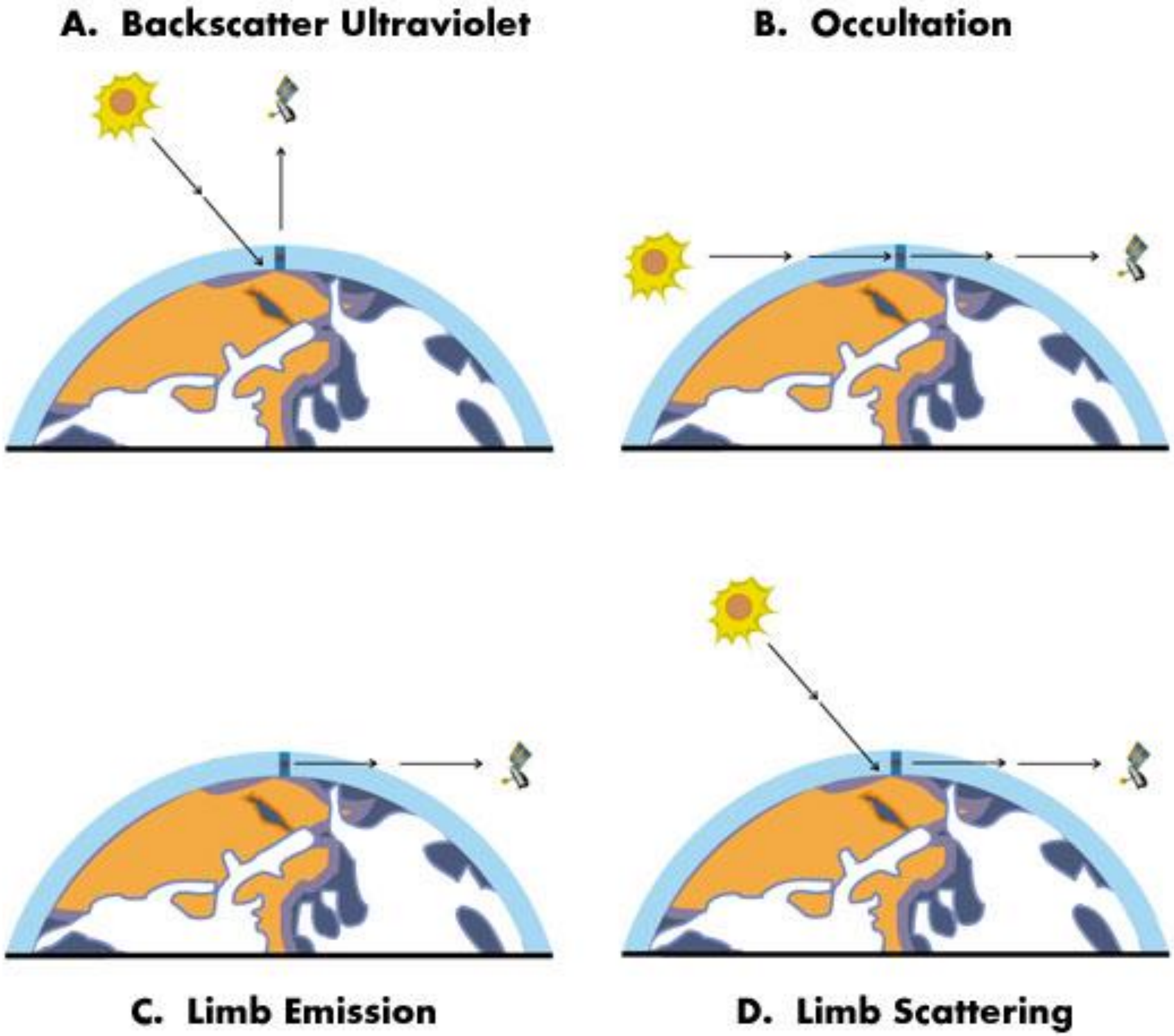
- *Relationship with SO_2*

  Expect SO_2 column to be derived accurately in TOMS V9

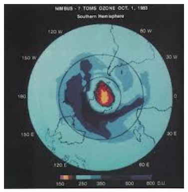
- *Learn more about the algorithm*

  Unique viewing conditions, potential Volcanic eruptions

Increased spatial and temporal resolution in GEO to provide more information and new opportunities (some yet unimagined).


A. Backscatter Ultraviolet
B. Occultation
C. Limb Emission
D. Limb Scattering

Current and Historical TOMS Missions



TOMS
Nimbus-7

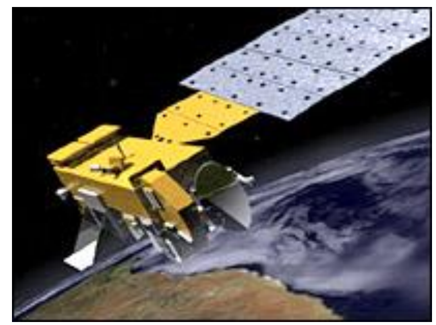
1978-1993

TOMS
Meteor-3

1992-1994

TOMS
EarthProbe

1996-2005



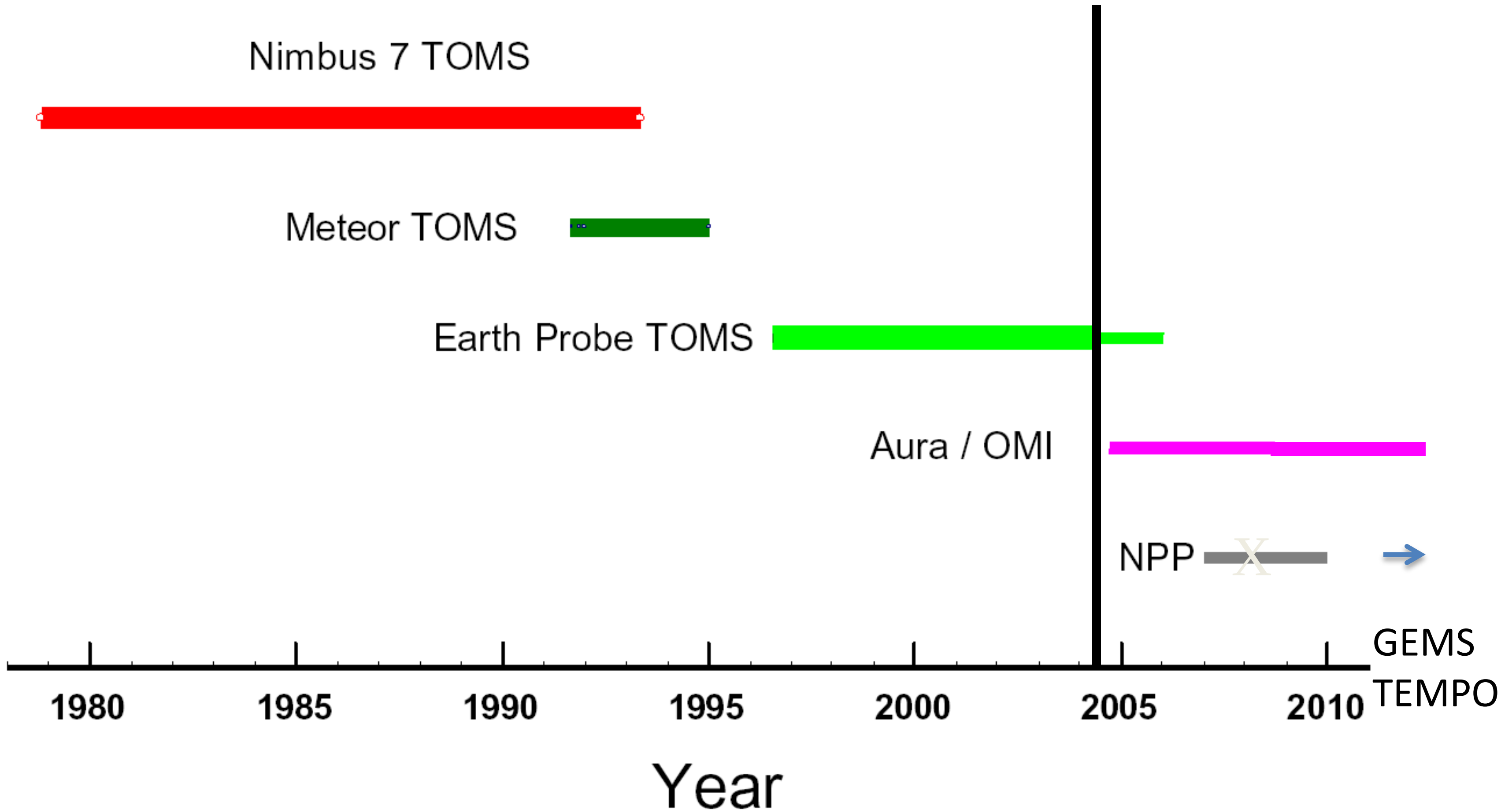
OMI
EOS Aura

2004 – pres.

OMPS
Suomi NPP

2011- pres.

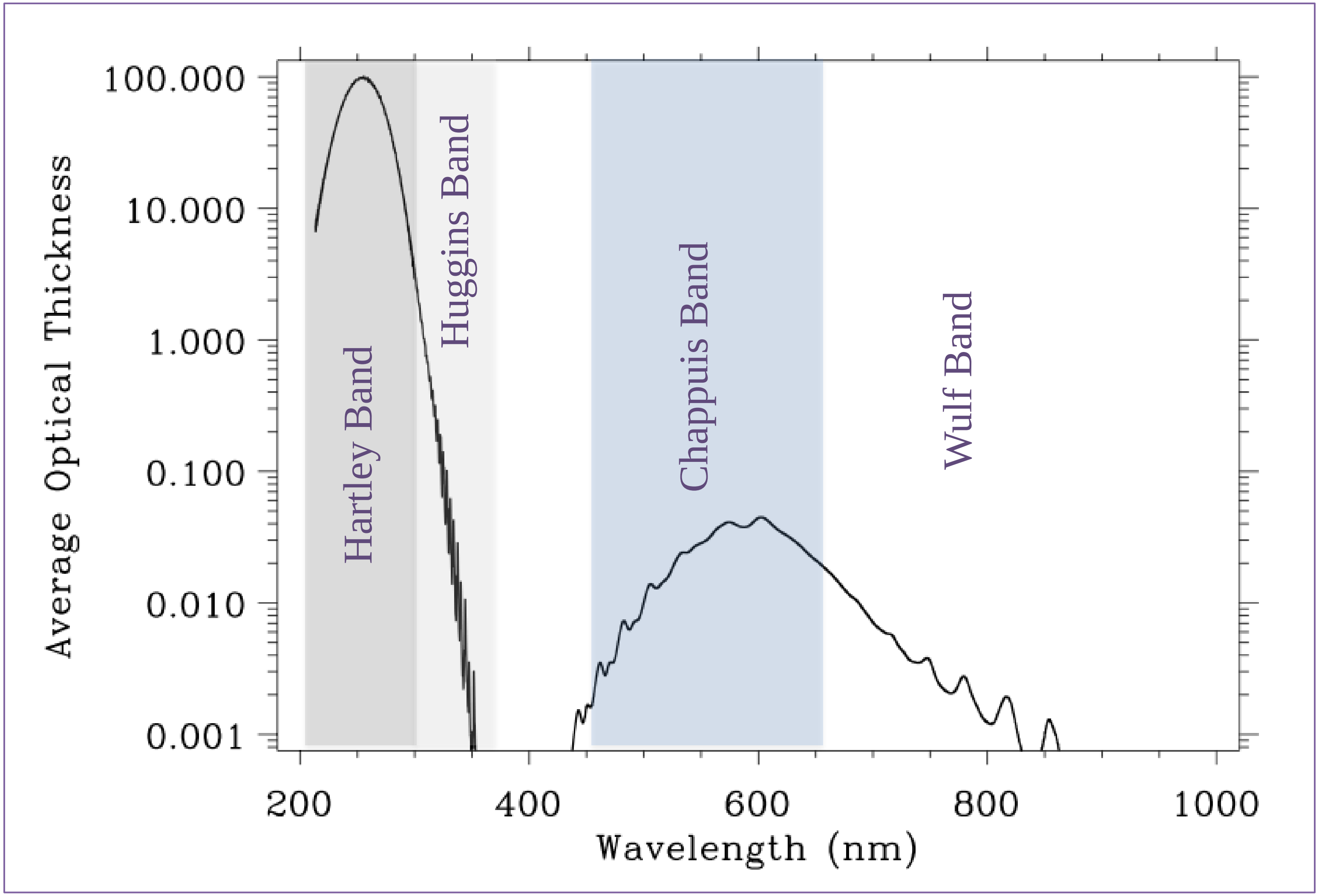
TOMS / Ozone Mapper Missions



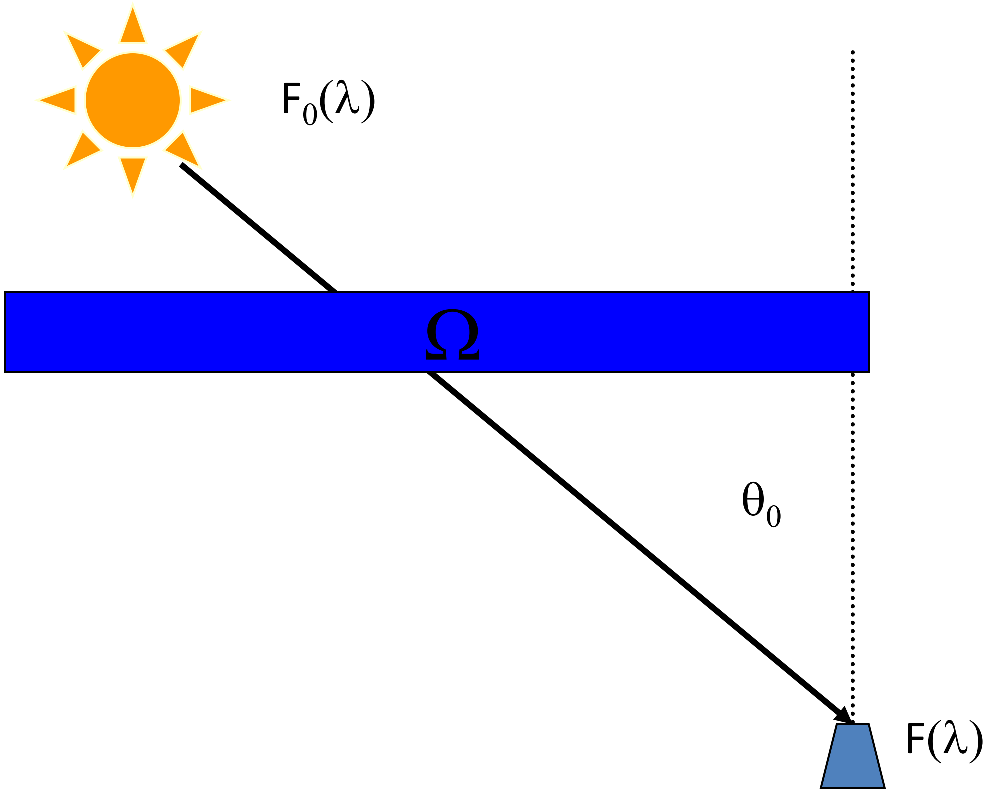
Backscatter UV Total O_3 Algorithms

Based on Dave & Mateer (1967)
SBUV V1-6 TOMS V1-8 OMI (NASA algorithm) Suomi/NPP OMPS Mapper (same as TOMS V8)
Spectral Fitting Algorithms
SBUV continuous scan (Joiner & Bhartia, 1997) GOME-DOAS OMI-DOAS WFDOAS BOAS BIRA/Direct Fit
Optimal Estimation Algorithms
GOME & OMI (Liu et al., 2005, 2010) SBUV V8.6 (Bhartia et al., 2012) Suomi/NPP OMPS NP (same as SBUV V8.6) TOMS V9 (similar to SBUV V8.6)

O_3 Absorption Optical Thickness



Effect of O_3 on transmitted flux



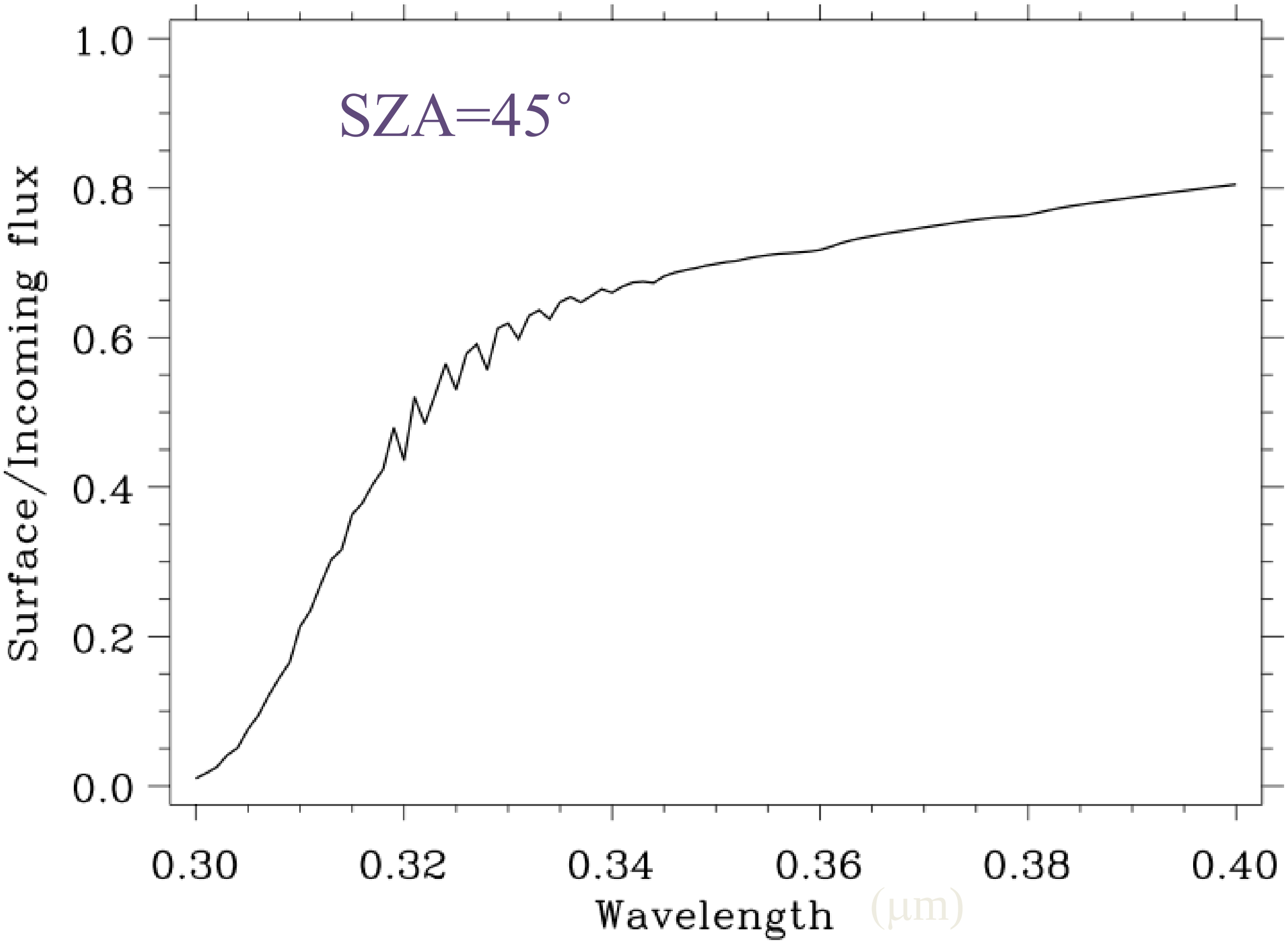
$T_{meas}(\lambda)=F(\lambda)/F_0(\lambda)$

$$T_{meas}(\lambda) = e^{-\mu\tau(\lambda)}$$

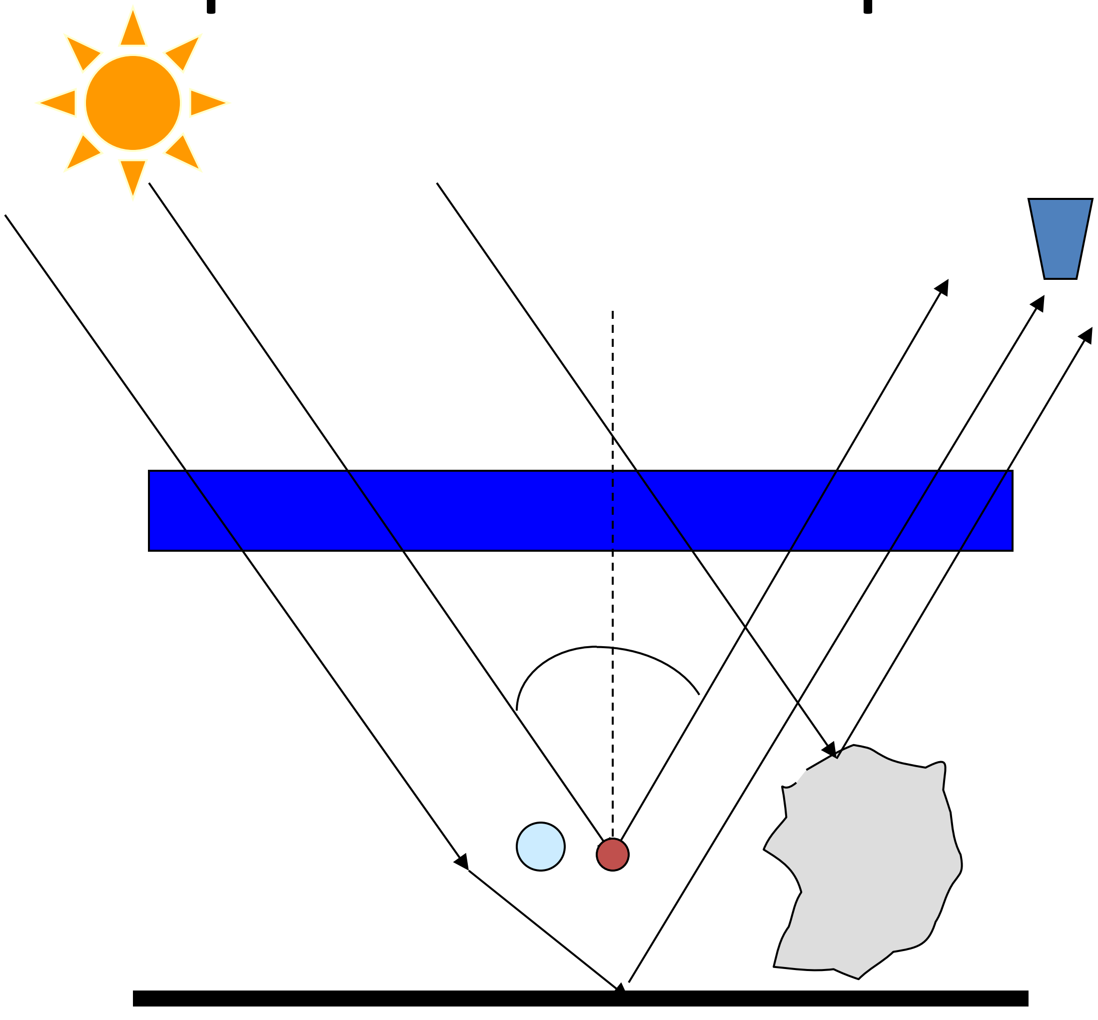
$$\mu \approx \sec\theta_0$$

$$\tau(\lambda) \approx \sigma_{o3}(\lambda)\Omega$$

How O_3 controls UV Radiation



Top-of-the-atmosphere Reflectance



TOA reflectance:

$$r(l) = \frac{pI(l)}{F_0(l)\cos q_0}$$

$$r(l) = r_0(l)e^{-mt_{O3}}$$

$$m \approx \sec q_0 + \sec q$$

$$t_{O3}(l) \approx s_{O3}(l)W$$

TOMS V9 algorithm Summary

- Primary objective is to provide error bars, and error kernels needed for estimating systematic errors.
- Secondary objective is to simplify the algorithm and extend retrievals to 88˚ SZA.
- No total O_3 will be provided in few % of cases where specialized algorithm is needed for data interpretation. These cases will be identified and radiances will be provided.

First Paper

JOURNAL OF THE ATMOSPHERIC SCIENCES

A Preliminary Study on the Possibility of Estimating Total Atmospheric Ozone from Satellite Measurements

J. V. DAVE AND CARLTON L. MATEER

National Center for Atmospheric Research, Boulder, Colo.

(Manuscript received 31 October 1966, in revised form 6 March 1967)

KEY IDEAS

- ***Use Ozone Profiles classified by total O_3***
- ***Treat Cloud and Aerosols as Opaque Lambertian Surface (LER model)***

Lambert-Equivalent Reflectivity (LER)

Assume that atmosphere is bounded by an opaque Lambertian surface at press p

$$I = I_0 + \frac{RT}{(1 - RS_b)}$$

LER $\rightarrow$

$$R = \frac{I - I_0}{T + (I - I_0)S_b}$$

Key Assumption: R doesn't vary with λ, so it can be derived from a non-O_3-absorbing λ and used at O_3 λs

- R is called Lambert-equivalent Reflectivity (LER)
- It is calculated from radiances measured at a weakly O_3- absorbing wavelength (330-380 nm).
- R is assumed to be the same at shorter O_3 sensitive wavelengths
- TOMS V9 algorithm: R accounts for surface, aerosol, clouds, and snow/ice (Dave and Mateer)

Issues with the LER model

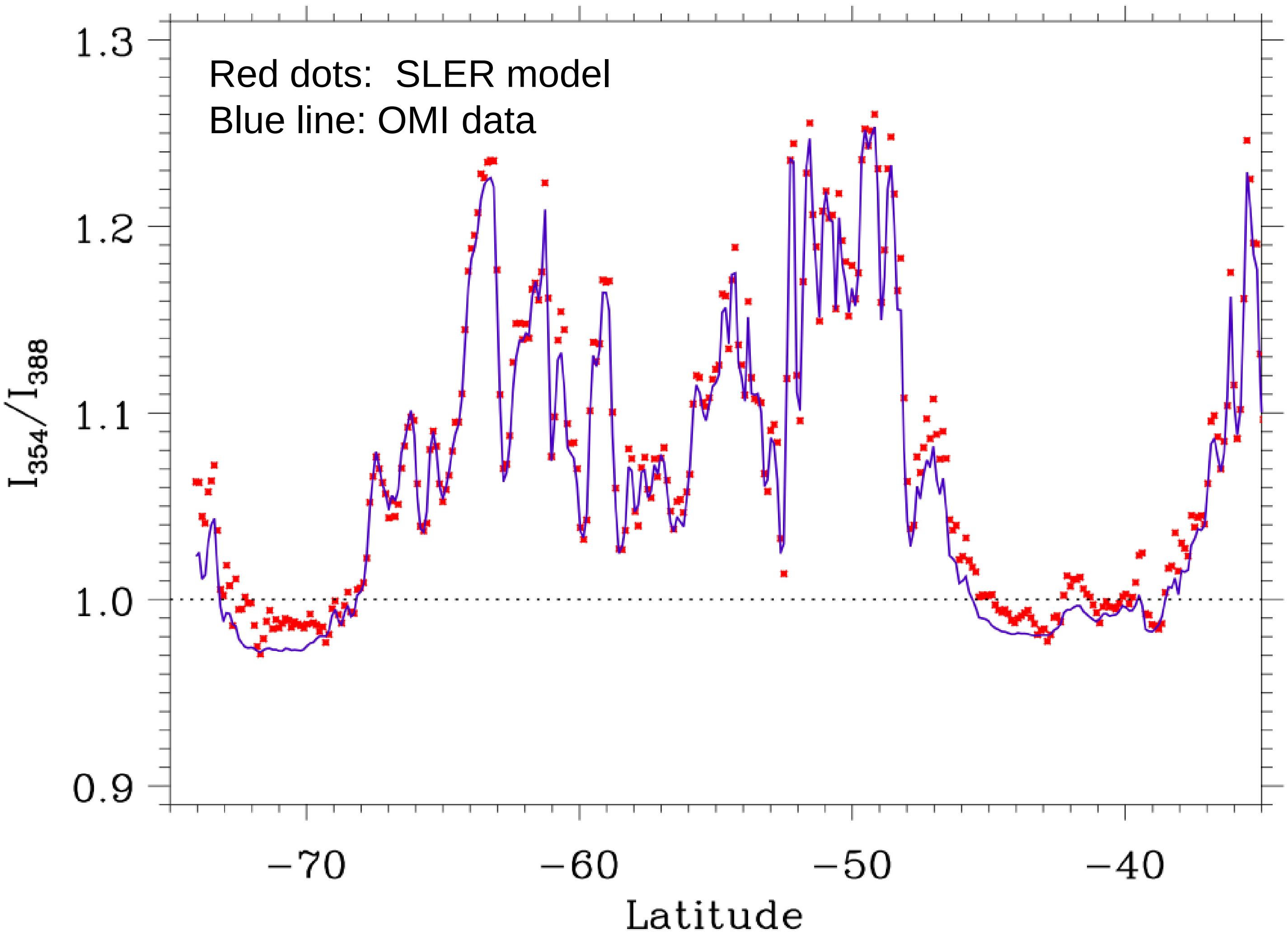
- LER of non-Lambertian surfaces varies with λ
  - Sea-glint is less bright at shorter λs due to diffuse light from Rayleigh
- LER of UV-absorbing aerosols decreases at shorter λ
  - Due to variation of AAOT with λ
- LER doesn't account for radiation that comes through the clouds
  - radiation is larger at shorter wavelenghts due to Rayleigh scattering below clouds

First two problems can be partially corrected by assuming LER varies linearly with λ

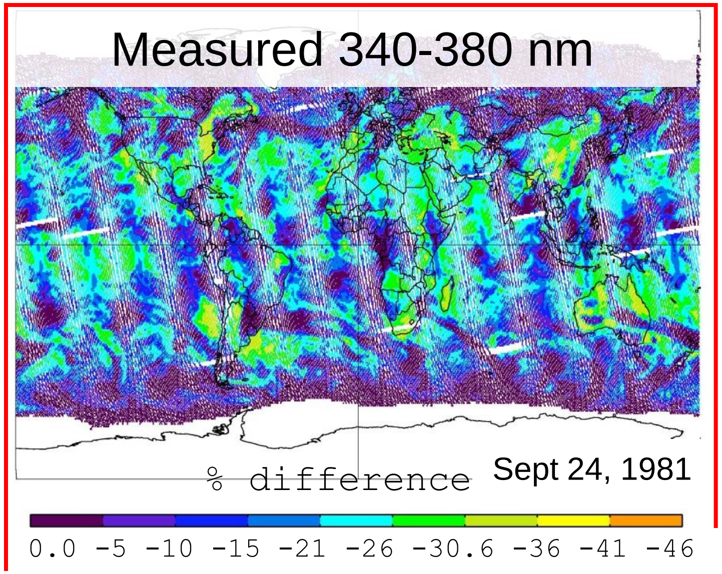
Strengths of SLER model

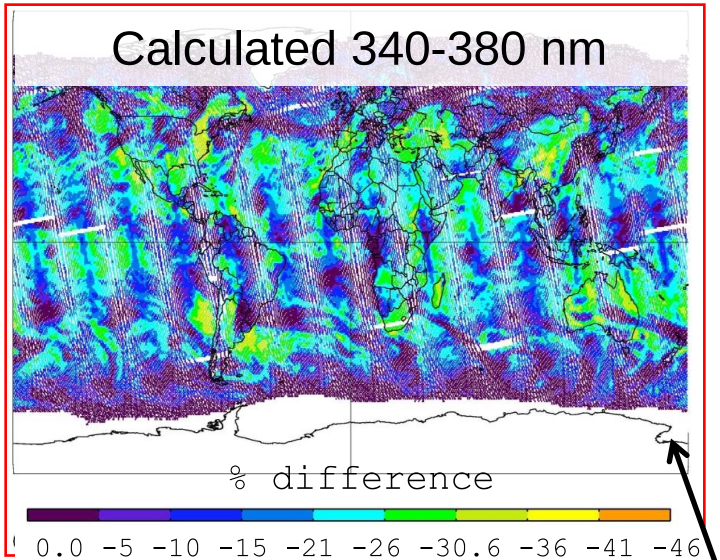
- Using just one parameter (R) it can model spectral dep of radiance due to Rayleigh scattering very well.
- An additional parameter (linear slope of R with λ) can account for aerosol absorption, terrain height, and non-Lambertian surfaces.
- Doesn't require knowledge of surface reflectivity, aerosols, cloud optical thickness, cloud fraction, cloud height or cloud type.

How well does SLER work?

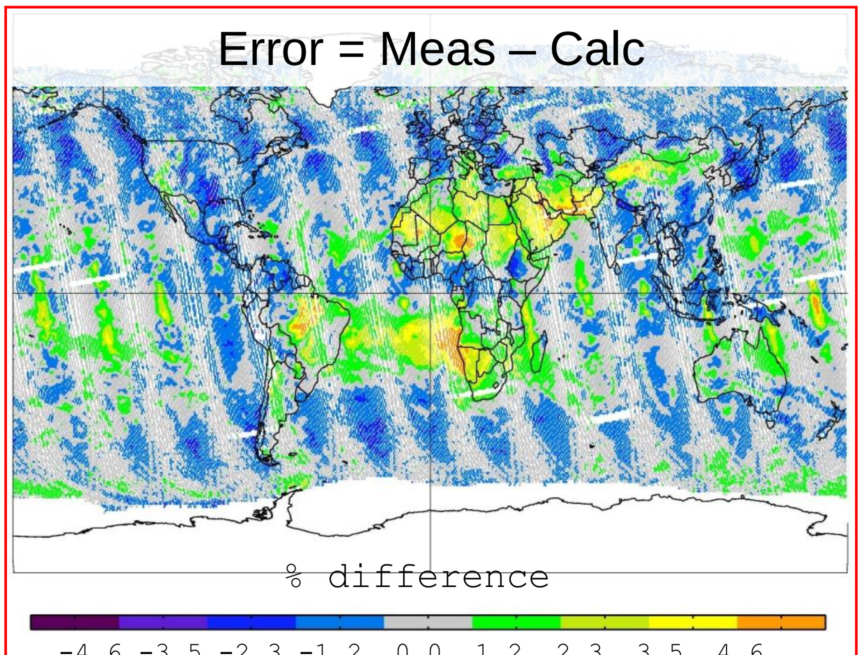


Percent difference in radiances from TOMS using LER





Pure LER model is used



Similar to AI

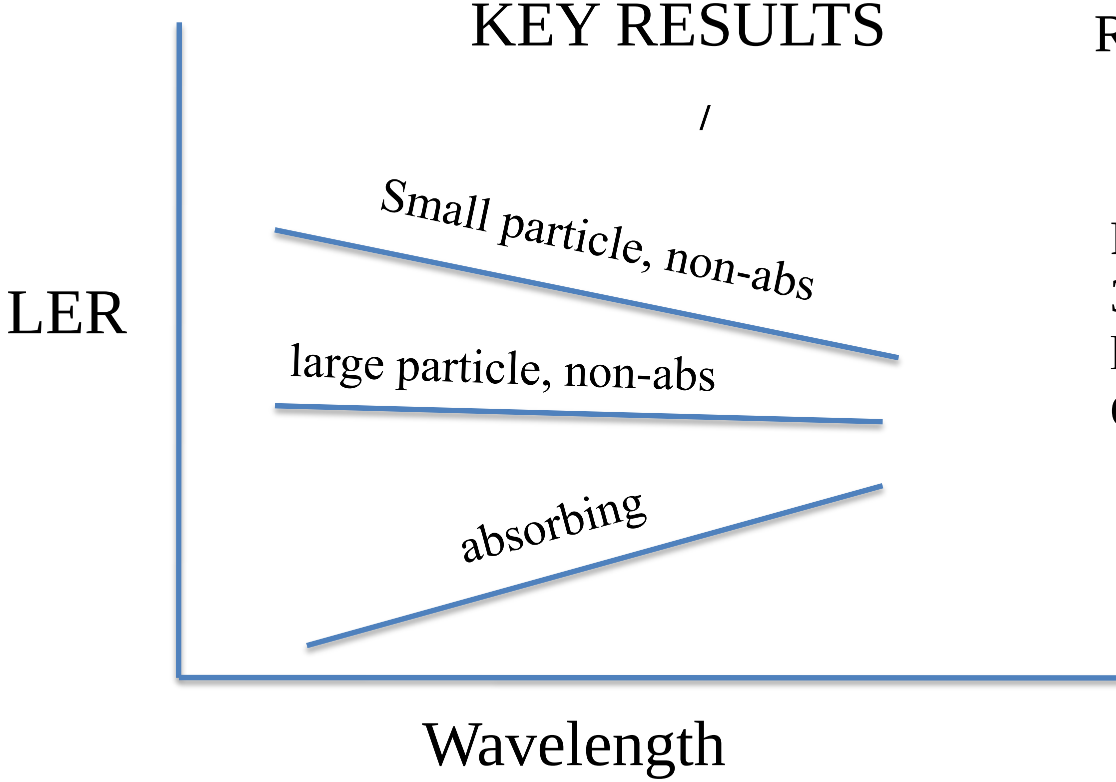
Effect of Aerosols on the Estimation of Total Ozone in an Atmospheric Column from the Measurements of Its Ultraviolet Radiance[1]

J. V. Dave

IBM Scientific Center, Palo Alto, Calif. 94304

(Manuscript received 17 November 1977, in final form 17 January 1977)

KEY RESULTS



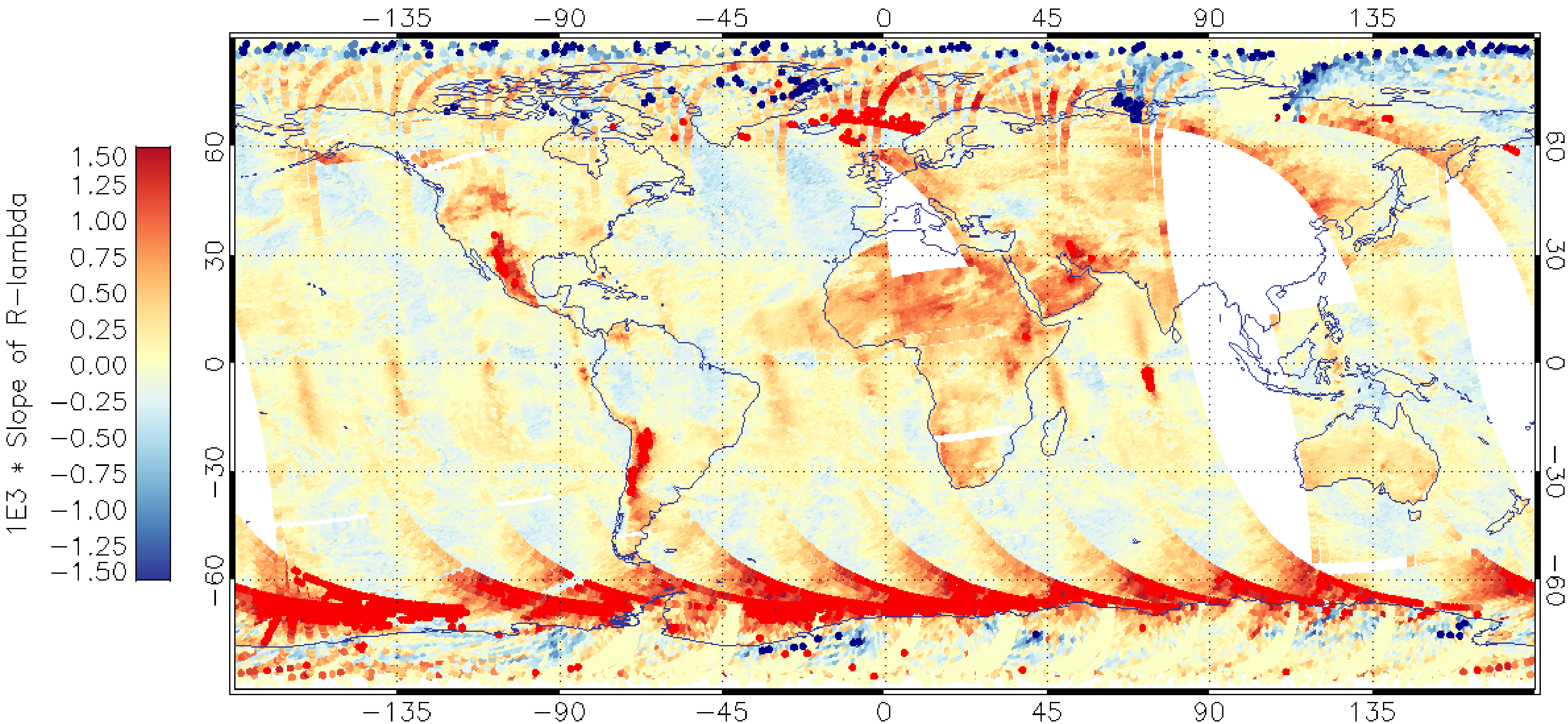
RECOMMENDATION

R could be measured at 340 and 380 nm and linearly extrapolated to O_3 wavelengths

Aerosol Correction

- If uncorrected, aerosol absorption appears as ozone enhancement.
- For low and moderate aerosol amounts, R-λ correction removes this effect
  - Retrieve LER at 340 and 380 nm
  - Linearly extrapolate R to O_3-absorbing λs
  - Retrieve O_3 with wavelength dependent R
- Approach fails for thick aerosols
  - Use more sophisticated correction or just flag data (not frequent).

Map of R-λ for SLER case

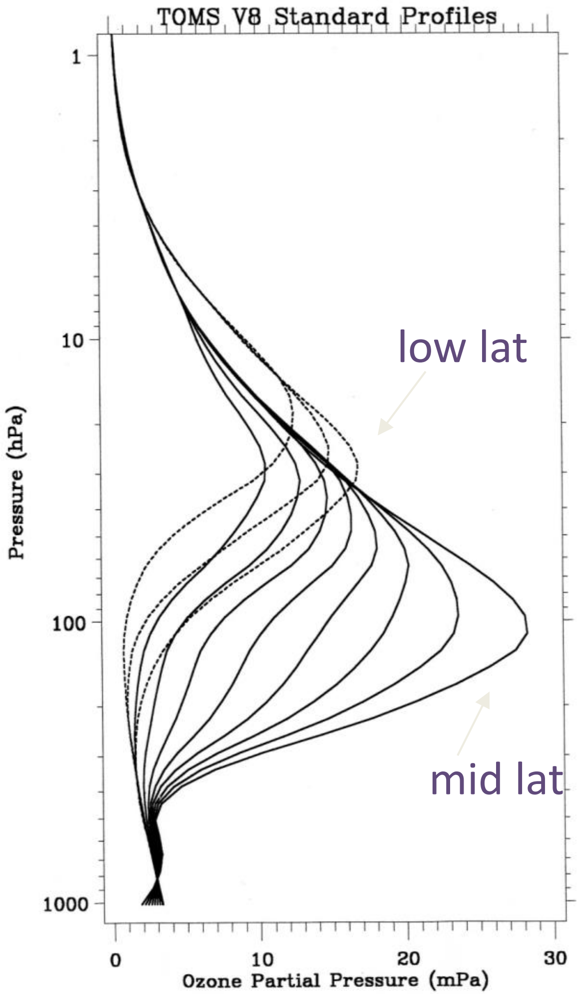


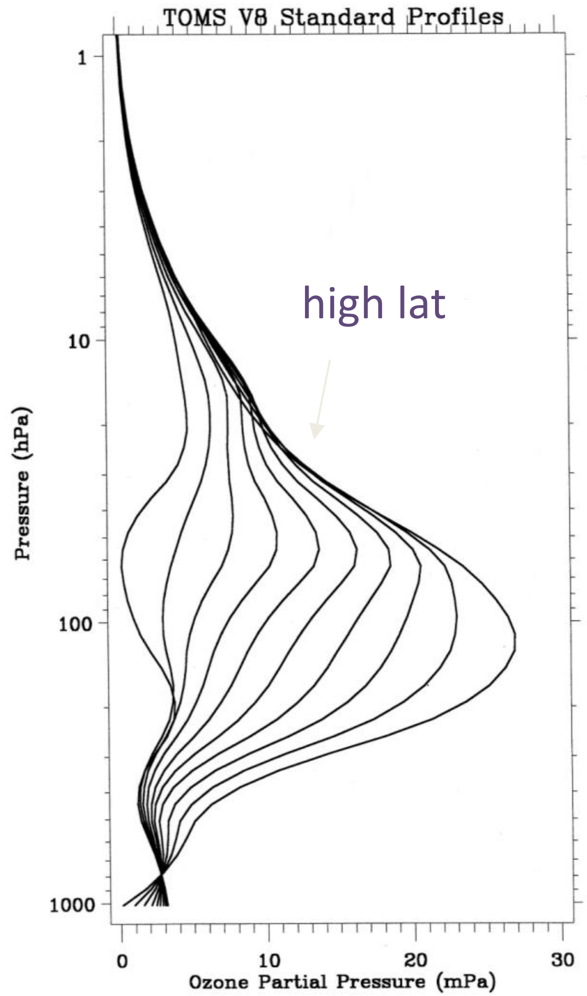
Sea Glint, High Terrain, Desert Dust all give pos. slope

Moderate → Linear; Extreme? Less likely

21 Standard O_3 Profiles

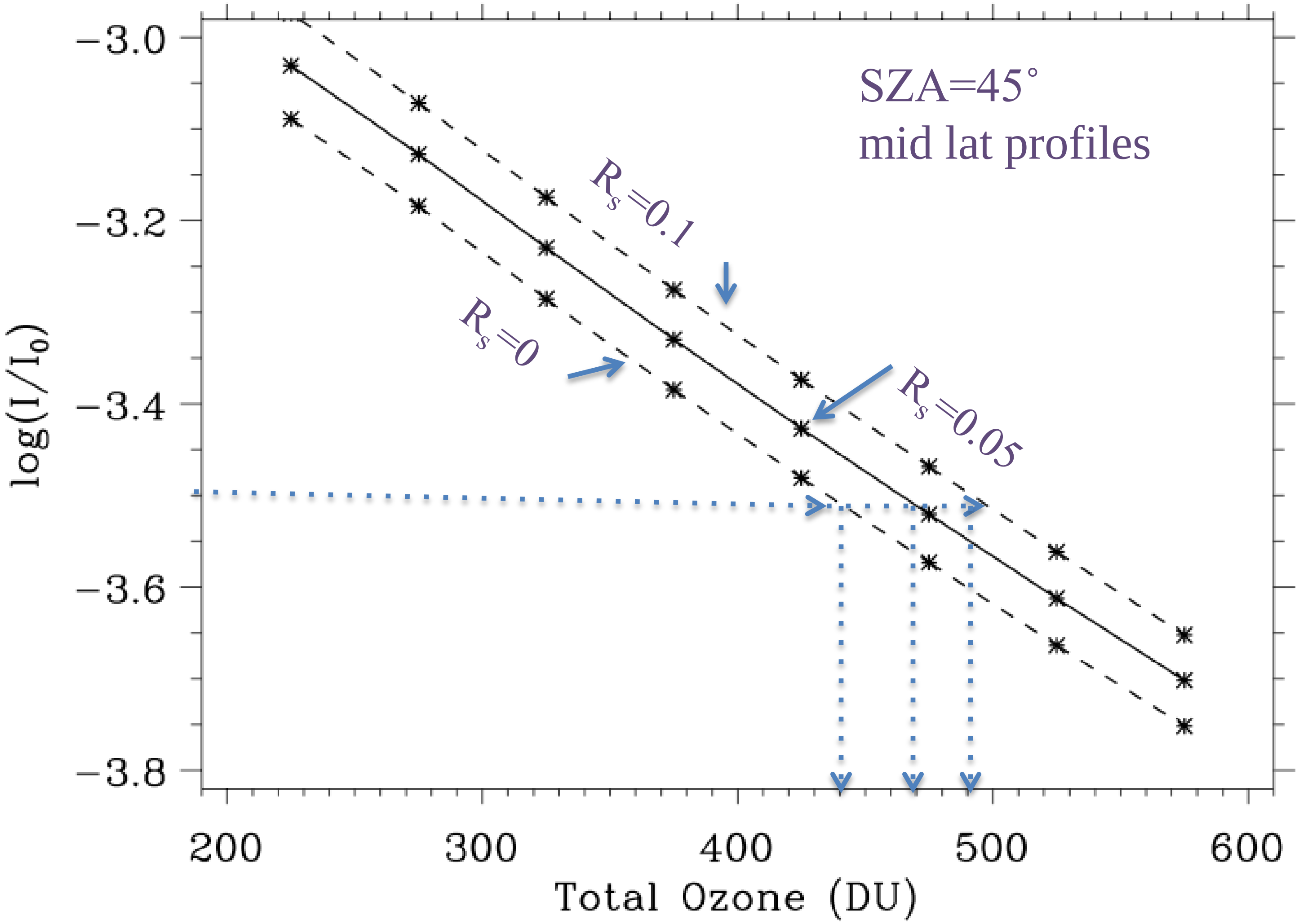
classified by total O_3 and lat band





$\log(I/I_0)$ vs Total O_3 at 317.5 nm

log I/I_0 vs Ω is almost linear at this SZA. Follows Beer-Lambert law approx.



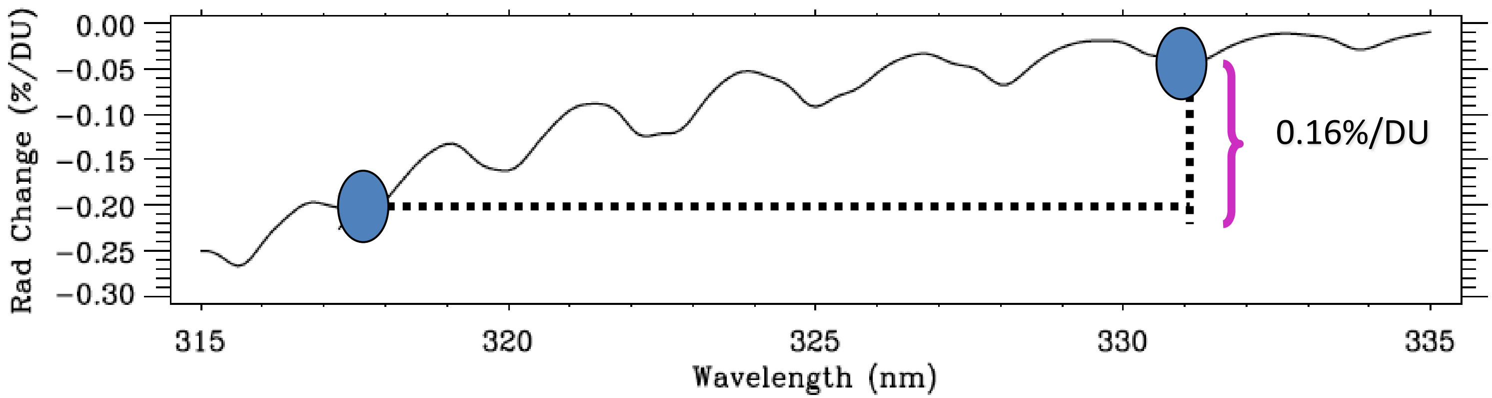
Can get different Ω depend upon R_s

TOMS wavelengths

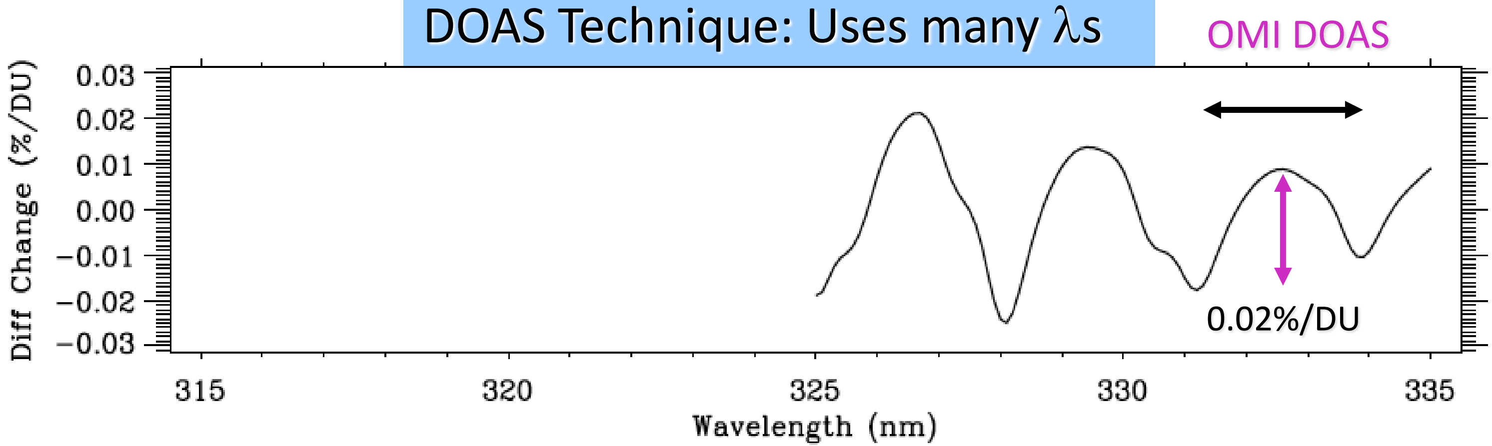
Nimbus-7 & Meteor	EP/TOMS
312.5	308.6
317.5	312.5
331.2	317.5
340.0	322.3
360.0	331.2
380.0	360.0

TOMS vs. DOAS

TOMS Technique: Uses 2 λs



DOAS Technique: Uses many λs



DOAS vs. TOMS- Differences

- TOMS algorithm works well with just 2 discrete λs with 300:1 signal/noise (S/N). DOAS requires ~100 wavelengths with at least 1000:1 S/N.
- DOAS is insensitive to calibration drifts that vary smoothly with λ, but it is very sensitive to high order drifts, TOMS is the opposite.
  - For both, calibration drift needs to be monitored by carefully examining the fitting residuals and other methods.

Ancillary Information

- Information needed to interpret a measurement
  - temperature, atmospheric pressure, absorption cross-section etc.
  - Such information is needed to interpret all types of measurements: laboratory, in-situ, and remote sensing
- Key difference is that *a priori* information refers to the variable one wants to measure, ancillary information to other variables.
  - e.g., to derive AOT from MODIS one needs cloud mask (ancillary information) and size distribution (*a priori* information).

A priori Information

- For our purpose it refers to the knowledge of a variable that exists BEFORE (prior to) one takes a measurement.
  - e.g., Based on past history, O_3 profile at Seoul today is n(z). The uncertainty is given by COV[n(z)].
- *A priori* knowledge is often necessary for deriving accurate results from remote sensing techniques.
  - *A priori* knowledge is not needed for in-situ techniques
  - Some remote sensing techniques require little or no *a priori* information, e.g., AOT from AERONET

What O_3 column satellites actually measure?

$$W_{actual} = \int_{z_s}^{\infty} w(z)n(z)dz \quad w(z) \neq 1 \text{ for all z}$$

$$\text{For thick clouds: } W_{actual} \; @ \int_{z_c}^{\infty} w(z)n(z)dz \quad w(z) \geq 1$$

$$W_{true} - W_{actual} = \int_{z_s}^{\infty} n(z)dz - \int_{z_s}^{\infty} w(z)n(z)dz = \int_{z_s}^{\infty} [1 - w(z)]n(z)dz$$

w(z) should be called Integrating Kernel. In TOMS algorithm it is called Efficiency Factor. Rodgers and Connor call it Column Averaging Kernel.

Citation: Rodgers, C. D., and B. J. Connor, Intercomparison of remote sounding instruments, *J. Geophys. Res.*, *108*(D3), 4116, doi:10.1029/2002JD002299, 2003.

How do we estimate total column O_3?

$$W_{retr} = \int_{z_s}^{\infty} w(z) n(z) dz + \int_{z_s}^{\infty} [1 - w(z)] n_{ap}(z) dz$$

$$W_{true} - W_{retr} = \int_{z_s}^{\infty} [1 - w(z)] \left[n(z) - n_{ap}(z) \right] dz$$

- Since $n(z)-n_{ap}(z)$ could be lot smaller than $n(z)$, we can reduce the error considerably by using *a priori* O_3 profile.
- Alternatively, we can provide *a priori* independent result by providing Ω_{actual}. But most users would not prefer this quantity, since it has no simple physical meaning.

Important Conclusions

- Remote sensing measurements often have missing information, e.g., ozone below clouds, or they have only partial information, e.g., lower atmospheric O_3 in clear sky.
- *A priori* information is used to provide the missing or partially missing information.
- It may be possible to provide a quantity that the satellite "actually" measured without using *a priori* information, but most users may not want such data.

Algorithm Components

X

↓

Forward Model

↓

I

↓

Inverse Model

↓

$\hat{X}$

$Y = F(X) + err$

dY/dX

Y = measurement vector (radiance, I)

X = state vector (Ω, n(z))

F = forward model fn. (RTM: VLIDORT, TOMRAD)

dY/dX = Jacobian (from RTM too.)

$X = F^{-1}(Y)$

Not perfect

(Ill constrained)

$\hat{X}$ = Retrieved profile

- Retrieval algorithm uses Inverse Model to estimate X from information contained in Y.
- Forward Model gives you tools to do so.
- You must supply a priori and ancillary data.

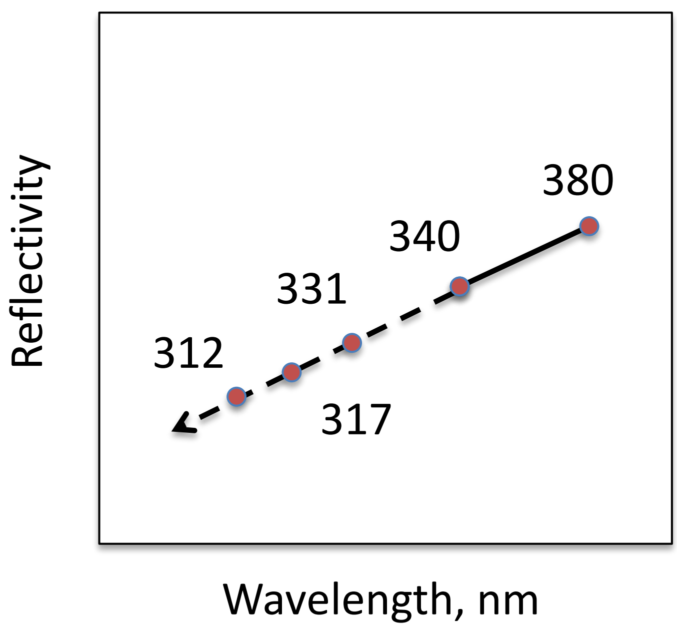
TOMS V9

Step 1	Calculate LER with linear R-λ assumption Calculate first guess O_3
Step 2	Perform retrieval (Optimal Estimation)
Step 3	Apply small correction for clouds

Step 1

Calculate LER with linear R-λ assumption

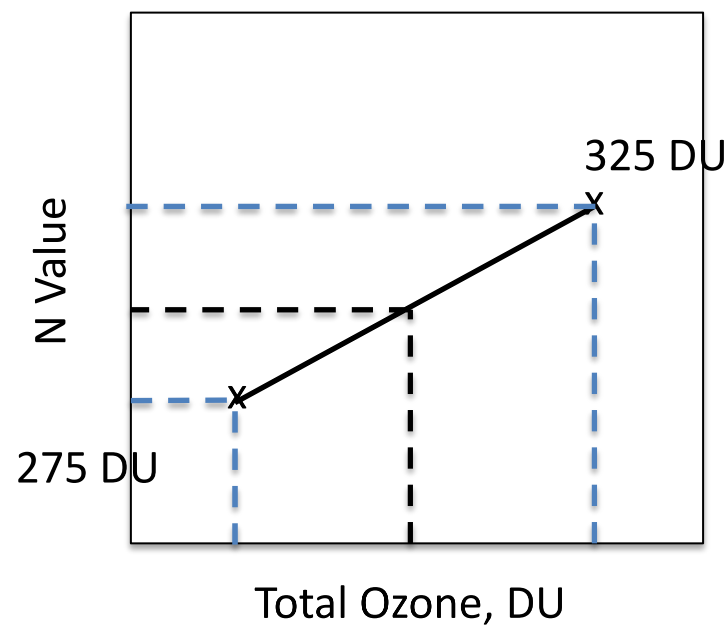
$$R = \frac{I - I_0}{T + (I - I_0) S_b}$$



Calculate first guess O_3

$$N = -100 \log I/I_o$$

317 nm



Step 2

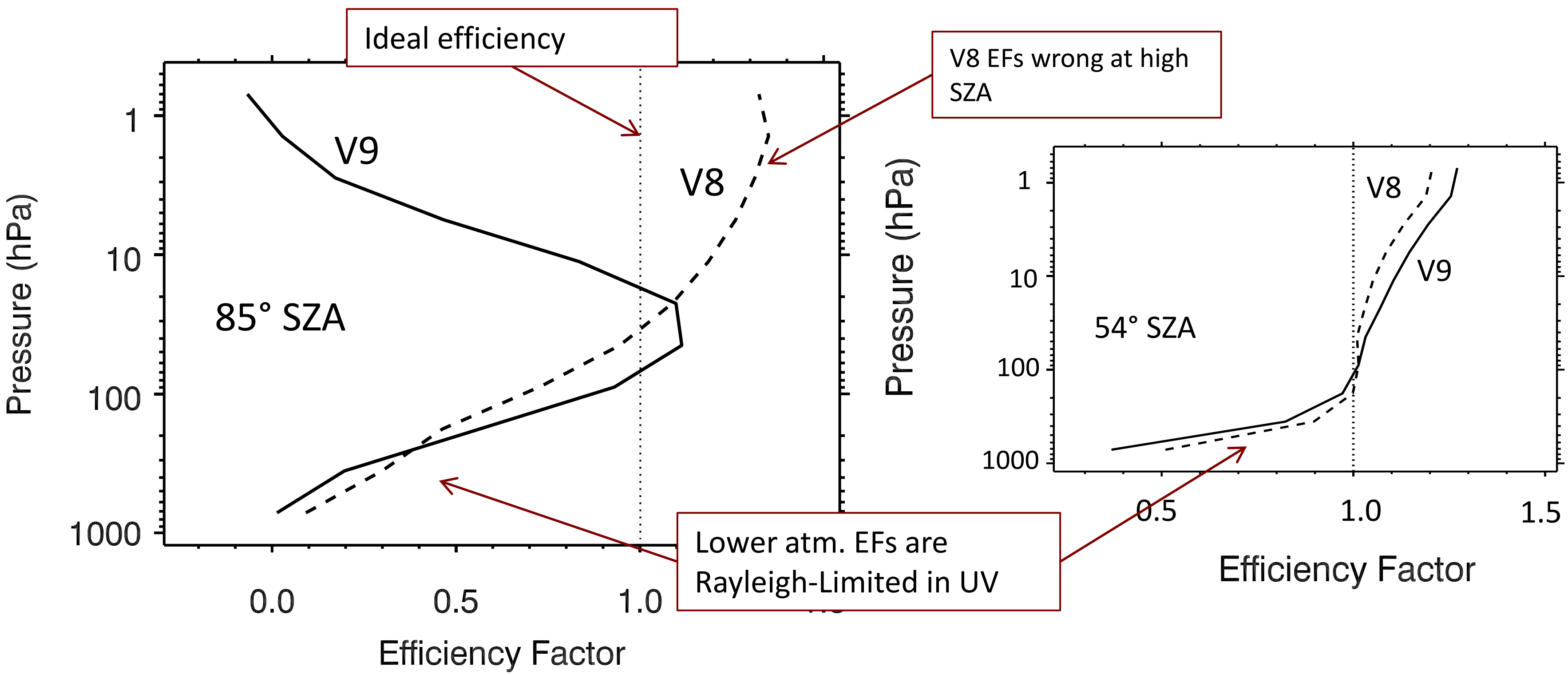
- Optimal Estimation a la Rodgers
- 3 Channels w/ O_3 sensitivity
  - 312, 317, 331
- 216 or dynamical profile *a priori* S_x
- Retrieval provides
  - Coarse Profile (11 layers) → Total O_3
  - Error
  - Integrating Kernel
  - Error Kernel
  - DFS

Role of S_x in Optimum Estimation

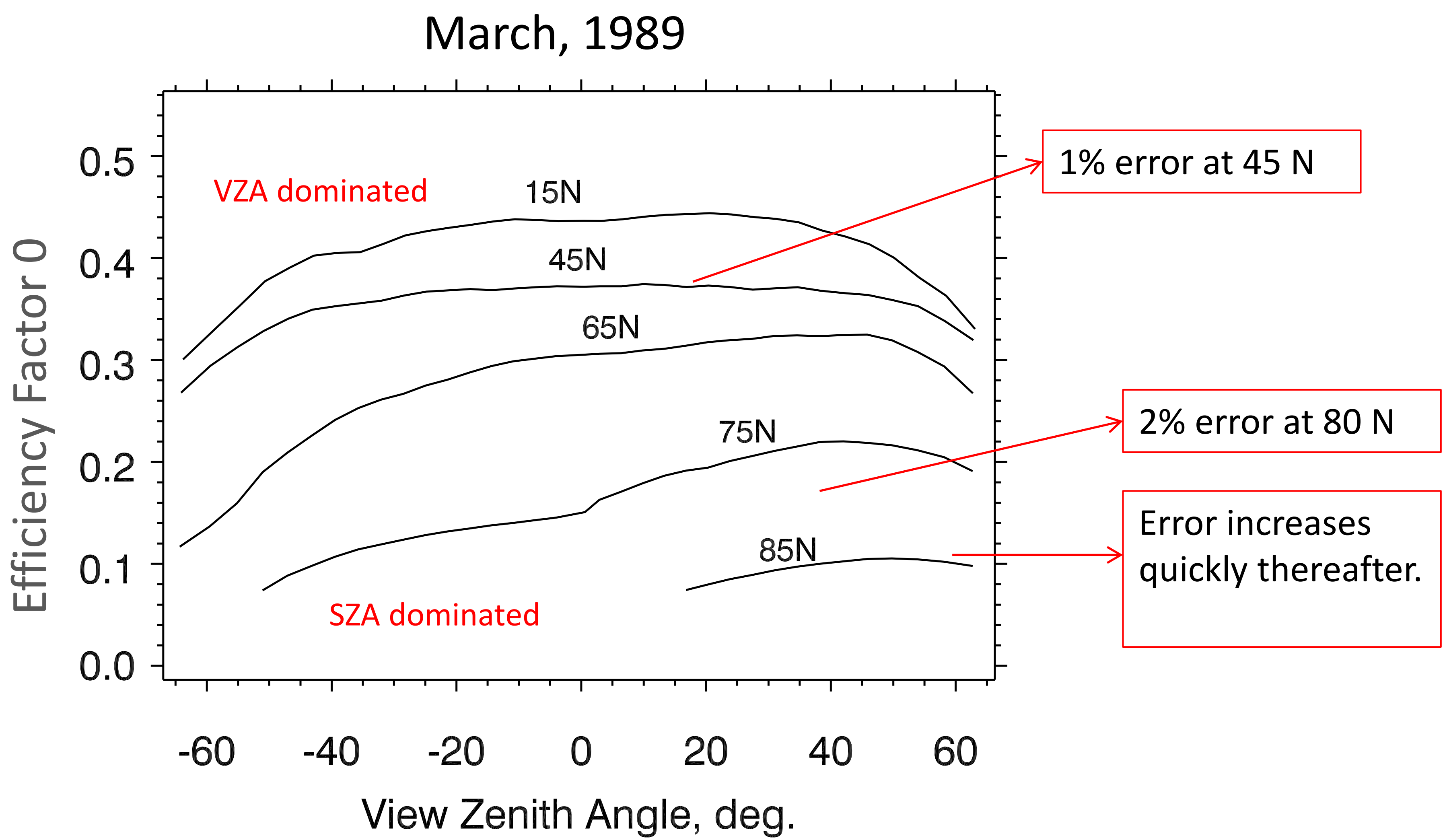
- Many people think of S_x as a constraint and make it arbitrarily large to minimize the impact of *a priori* on the retrieved profile. This is a mistake.
- The purpose of S_x is to help you select the best (i.e., statistically most probable) profile from many possible profiles, all of which can explain the measurements to within the measurement error prescribed by the S_e matrix.
- At least the diagonal elements of S_x should be derived from real data with vertical resolution higher than the one we are retrieving. For the BUV technique, MLS and ozonesondes provide the best data to construct $S_{x.}$.

TOMS Efficiency Factors

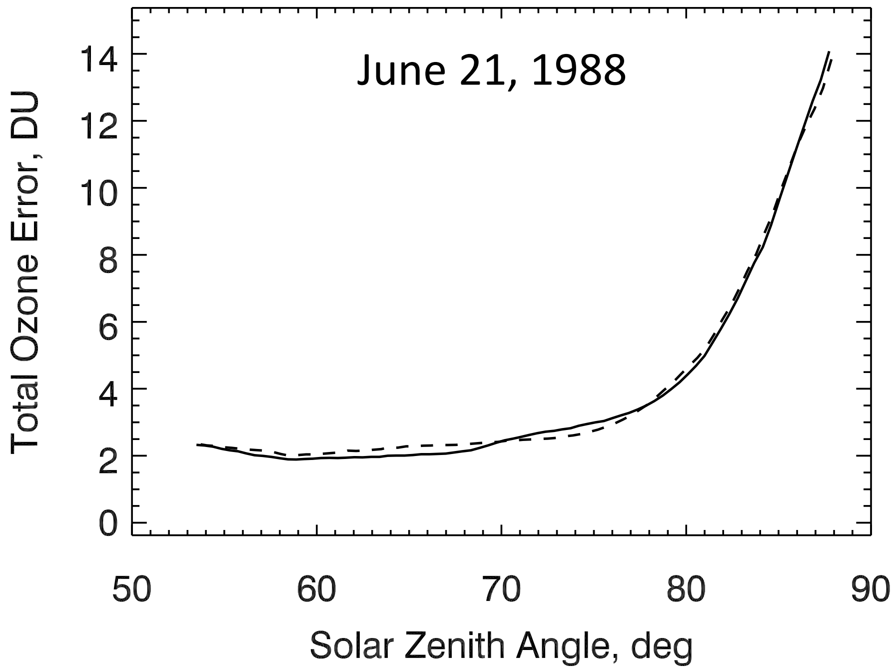
Integrating Kernel (IK)	→	Column Integrating Kernel (CIK)	→	Efficiency Factors (EF)
$\mathbf{W} = \mathbf{S}_x \mathbf{K}_1^T (\mathbf{K}_1 \mathbf{S}_x \mathbf{K}_1^T + \mathbf{S}_e)^{-1} \mathbf{K}_1$		$\mathbf{W}^C = \sum_i w_{ij}$		w_j^C
(a.k.a. Averaging Kernel)		sum over columns of IK		elements of CIK



Overall Geometry Dependence of Error

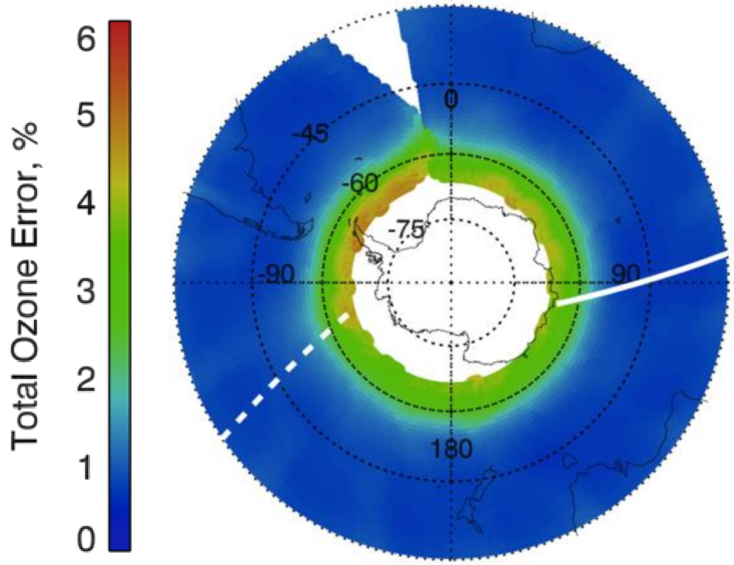


Error Dependence with SZA

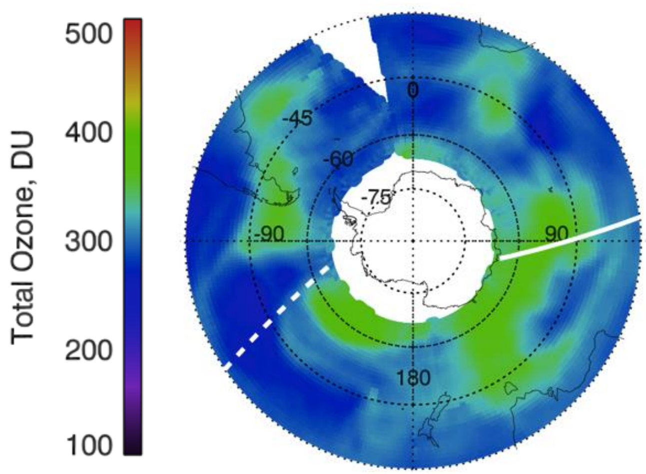


- Error varies by factor of 10.
- Most dependence is w/ SZA, not O_3, VZA.
- Reason: EFs reduce dramatically in lower atmosphere as path length increases.
- Less info. from measurements → greater reliance on *a priori* → larger uncertainty.

Column Error

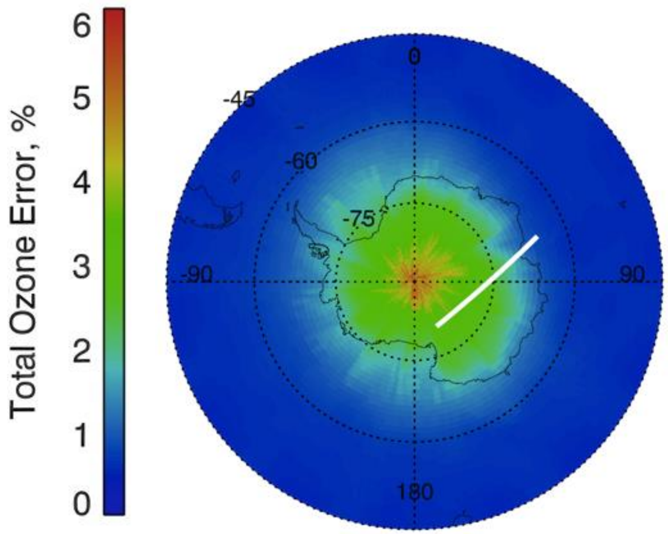


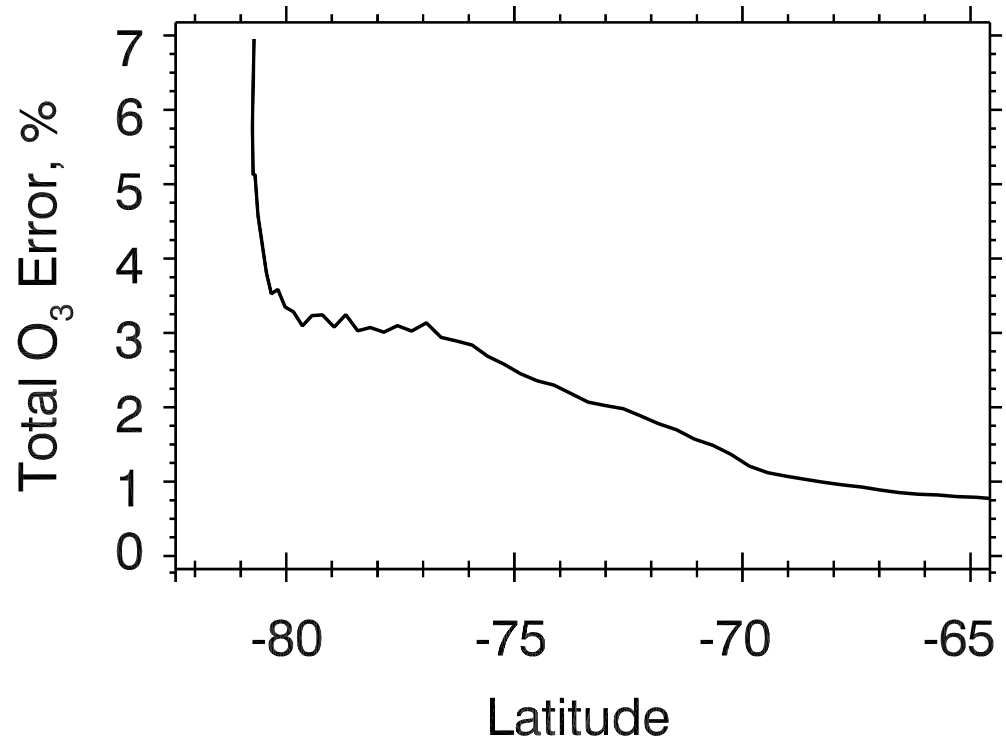
Column Amount



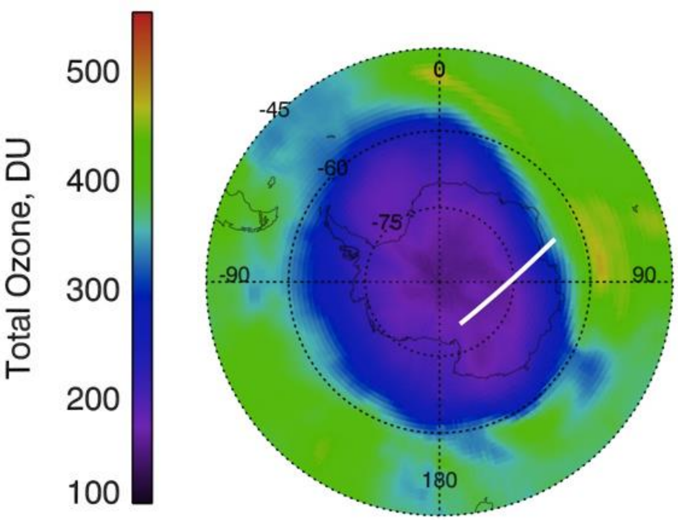
Error Bars for O_3 Hole Conditions

Column Error in Sep 29, 1987 Ozone hole





Column Amount



- Errors increase sharply at high SZA
- With error bars we can properly qualify measurements made at extreme SZA.
- Errors are important to consider when tracking ozone minima.

Step 3

- A very small adjustment to the total column
- Why so small?

Come this afternoon to cloud tutorial!

References

- Dave, J.V., and Mateer, C. L.: A Preliminary Study on Possibility of Estimating Total Atmospheric Ozone from Satellite Measurements, J. Atmos. Sci., 24, 414-427, 1967.
- Joiner, J. and Bhartia, P.K.: Accurate determination of total ozone using SBUV continuous spectral scan measurements, J. Geophys. Res.-Atmos., 102, 12957-12969, 1997.
- Liu, X., Chance, K., Sioris, C.E., Spurr, R.J.D., Kurosu, T.P., Martin, R.V., and Newchurch, M.J.: Ozone profile and tropospheric ozone retrievals from the Global Ozone Monitoring Experiment: Algorithm description and validation, J. Geophys. Res.-Atmos., 110, D20307, doi:10.1029/2005JD006240, 2005.
- Liu, X., Bhartia, P.K., Chance, K., Spurr, R.J.D., and Kurosu, T. P.: Ozone profile retrievals from the Ozone Monitoring Instrument, Atmos. Chem. Phys., 10, 2521-2637, 10.5194/acp-10-2521-2010, 2010.
- Bhartia, P.K., McPeters, R.D., Flynn, L.E., Taylor, S., Kramarova, N.A., Frith, S., Fisher, B., and Deland,M.: Solar Backscatter UV (SBUV) total ozone and profile algorithm, Atmos. Meas. Tech. Discuss., 5, 5913-5951, doi:10.5194/atmd-5-5913-2012, 2012.
- Dave, J. V., Effect of Aerosols on Estimation of Total Ozone in an Atmospheric Column from Measurements of Its Ultraviolet Radiance, J. Atmos. Sci., 35, 809–911, 1978.