Modeling Processes

Case Study of a Dust Storm

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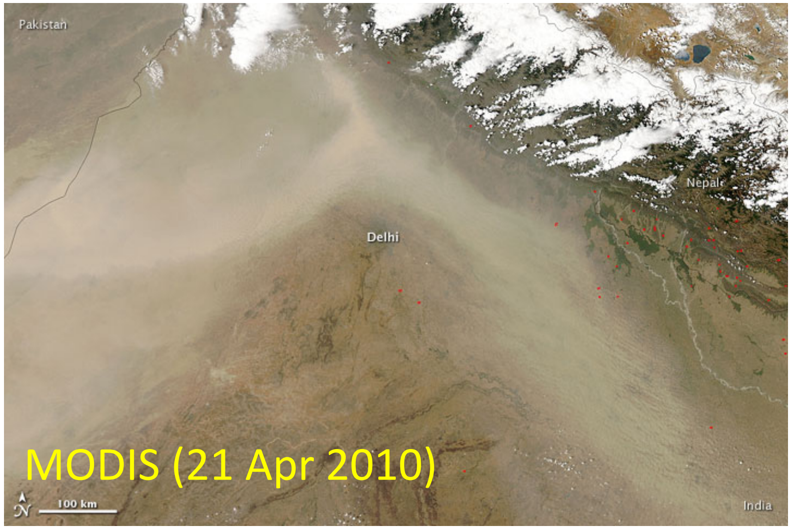
Kumar et al. (2014) *Atmos. Chem. Phys.*, Dust effects on radiation and aerosol optical properties

Kumar et al. (2014) *Atmos. Chem. Phys.,* Dust effects on chemistry

Exercises will be on these topics:

1. Calculation of photodissociation rate constants
2. Effects of aerosols on photodissociation rate constants

Why Model Dust Storms and Chemistry?

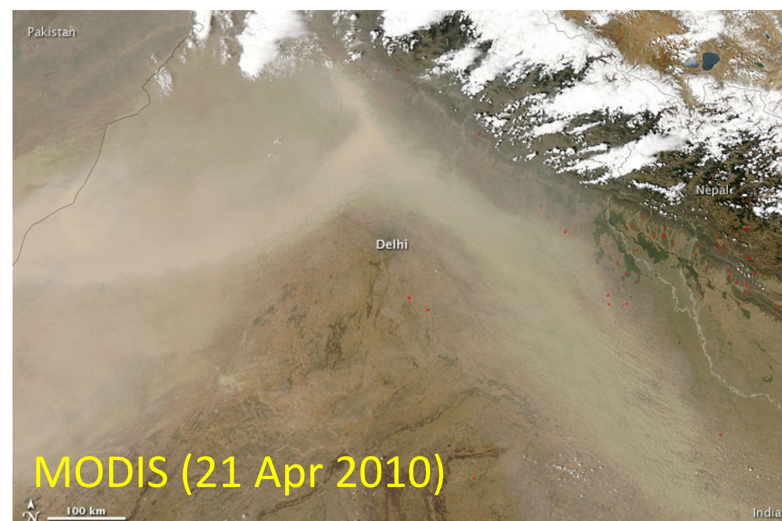


- Dust storms often occur during the pre-monsoon (MAM) season in northern India and affect day to day life.

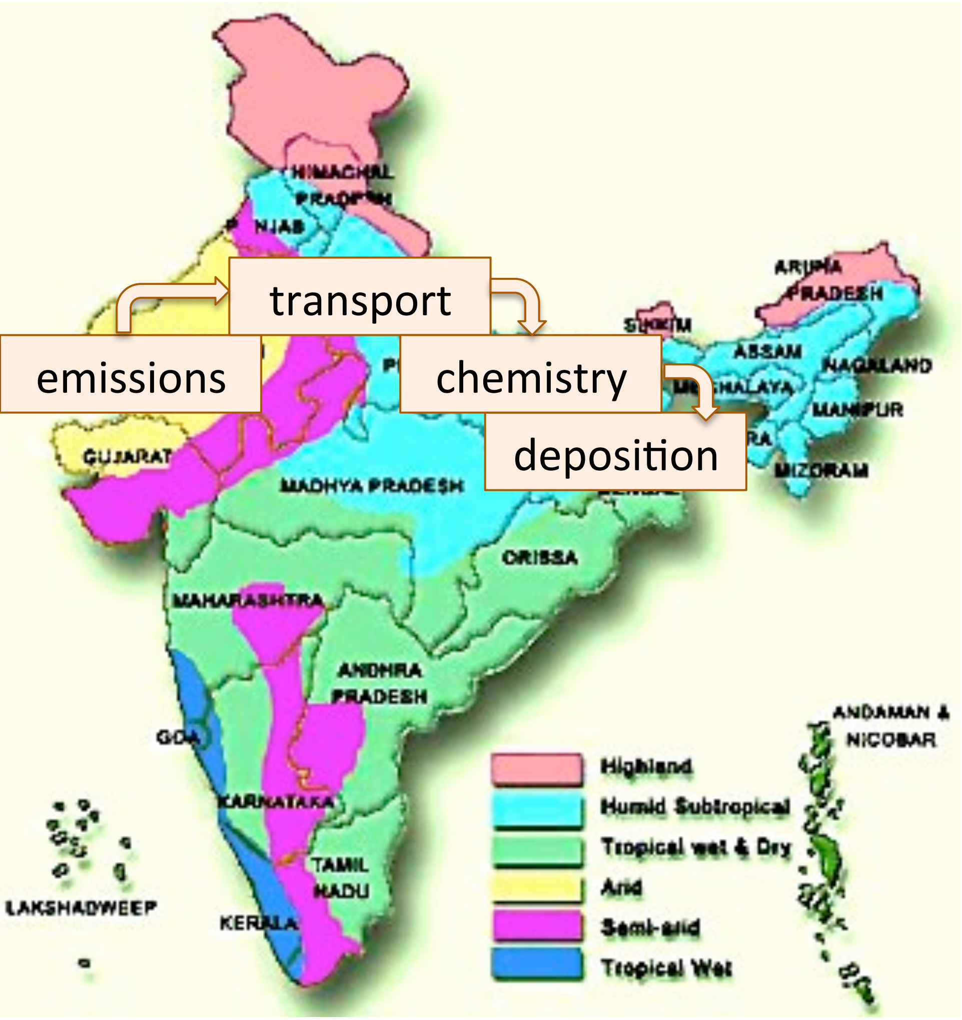
- **GOAL:** Understand the effect of these dust storms on regional scale aerosol optical properties, radiation budget and tropospheric chemistry.

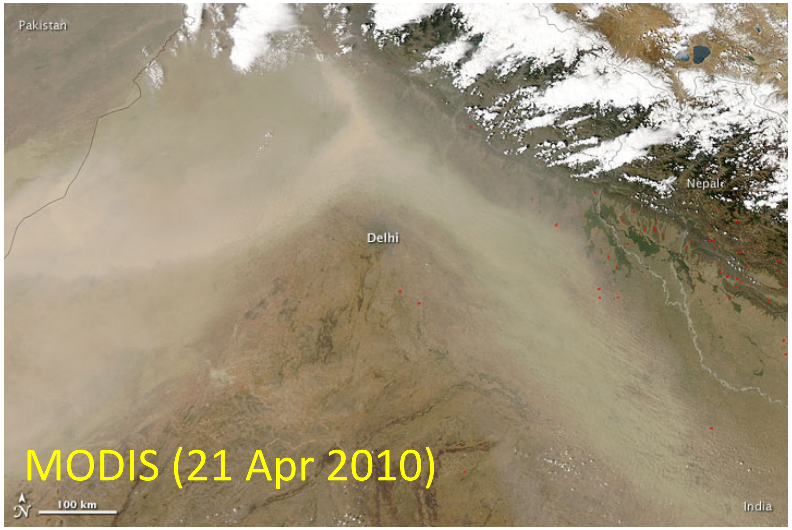
What Causes the Dust to Reside over the IGP?

Dust from the Thar Desert gets channeled by the topography of the Indo-Gangetic Plain



What Processes Happen from the Desert to the IGP?





Modeling dust storm effects on aerosols and trace gases

- Emissions
  - Dust emissions = f(wind, soil type & moisture)
  - Sea salt emissions = f(wind)
  - Anthropogenic emissions = prescribed
  - Biomass burning emissions = f(fire size, vegetation)
  - Emissions from vegetation = f(vegetation type, T, PAR)
- Transport
- Chemistry
- Deposition

Modeling emissions of aerosols and trace gases

- Dust Emissions

$$Dust_{emis} = C\,(f_{size} \times erod \times area)\,(wspd_{10m})^2\,(wspd_{10m} - u_{thres})\,dt$$

C = tuning factor

→ *Improving dust emissions for different deserts is important*

- Sea Salt Emissions

$$SS_{emis} = 4/3(\pi\,(r_{dry})^3\,\rho_{SS}\,frh\,dF_n\,dr)\,dt$$

These equations are from the WRF-Chem GOCART emissions modules. They can easily vary among models. References are Ginoux et al. (2001, 2004); Chin et al. (2002).

Modeling emissions of aerosols and trace gases

- Anthropogenic Emissions
  - Several emissions inventories available
  - See ECCAD web site ***eccad****.sedoo.fr/* and Sachin Ghude's lecture
- Biomass Burning Emissions

  GFED *www.globalfiredata.org/*

  QFED http://gmao.gsfc.nasa.gov/research/science_snapshots/global_fire_emissions.php

  FINN https://www2.acd.ucar.edu/modeling/finn-fire-inventory-ncar

  Forecast http://www.acd.ucar.edu/acresp/forecast/fire-emissions.shtml
- Biogenic Emissions

  MEGAN
  https://www2.acd.ucar.edu/modeling/model-emissions-gases-and-aerosols-nature-megan

  BEIS
  http://www.epa.gov/ttn/chief/emch/biogenic/beis/index.html

Modeling transport of aerosols and trace gases

- Emissions
- Transport
  - Resolved on grid of model
  - Parameterized motions in the boundary layer (i.e. diffusivity to represent large eddy motions)
  - Parameterization of convective transport
- Chemistry
- Deposition

Modeling transport of aerosols and trace gases

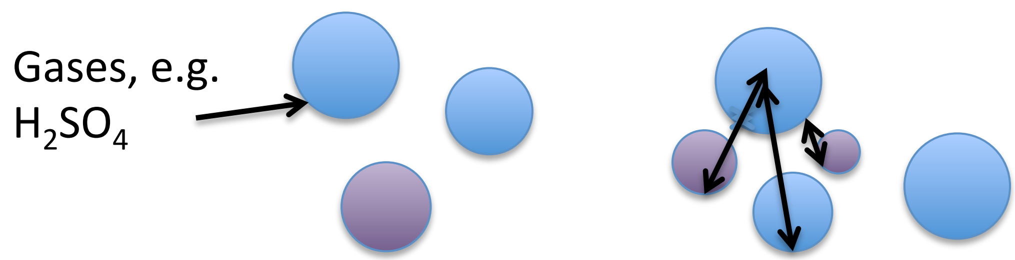
- Transport
  - See lectures by Mark Lawrence and Federico Fierli

Modeling chemistry of aerosols and trace gases

- Emissions
- Transport
- Chemistry
  - Aerosol growth by condensation and coagulation
  - Photodissociation reactions
  - Reactions between trace gases
  - Reactions between gas and aerosol
  - Reactions in cloud and rain drops
- Deposition

Modeling aerosol physics and chemistry

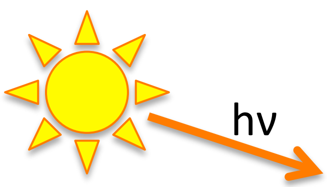
- Aerosol growth by condensation and coagulation



- Photodissociation reactions
- Reactions between trace gases
- Reactions between gas and aerosol
- Reactions in cloud and rain drops

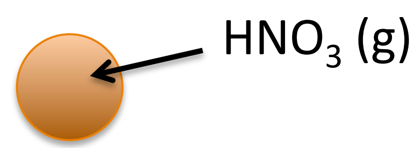
Modeling chemistry of aerosols and trace gases

- Aerosol growth by condensation and coagulation
- Photodissociation reactions



$NO_2 \rightarrow NO + O$

- Reactions between trace gases, e.g. $NO + O_3 \rightarrow NO_2$
- Reactions between gas and aerosol



HNO_3 (g) + dust $\rightarrow$ 0.5 NOx

- Reactions in cloud and rain drops

e.g. $HSO_3^- + H_2O_2 \rightarrow SO_4^{2-}$

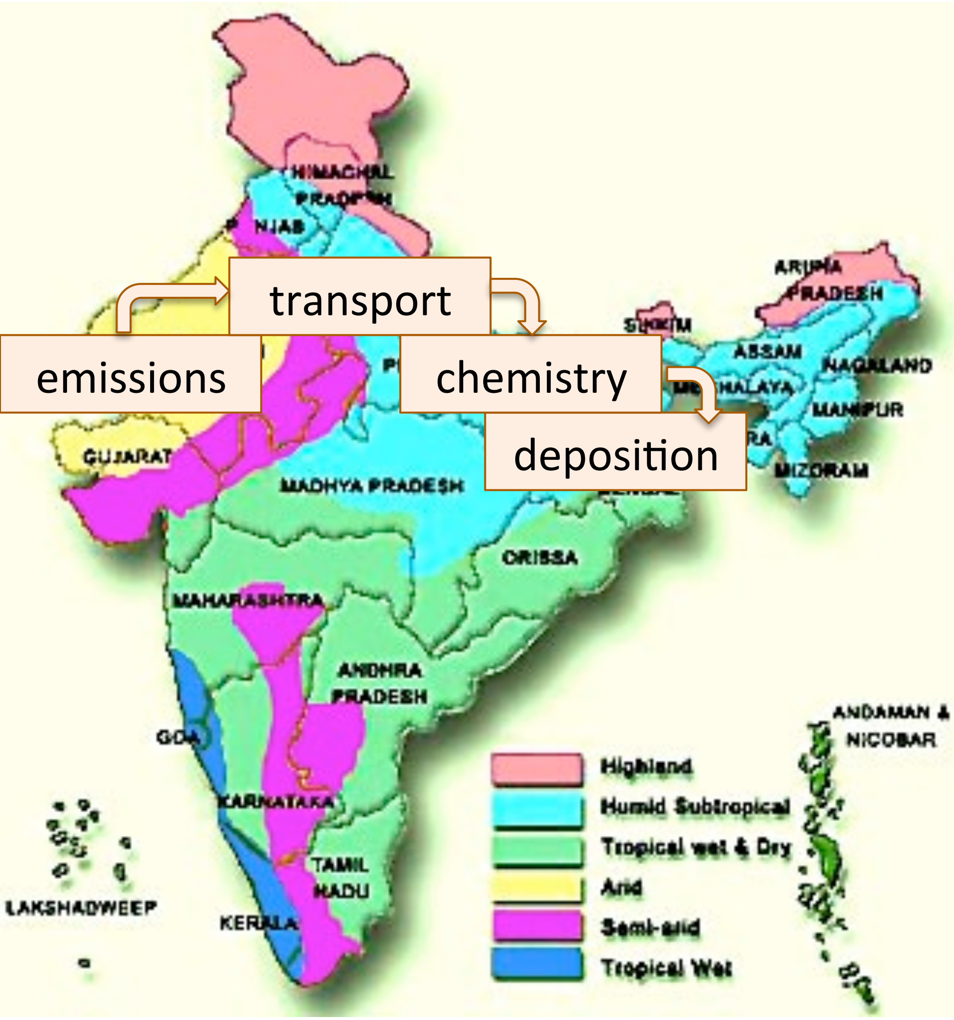
Modeling deposition of aerosols and trace gases

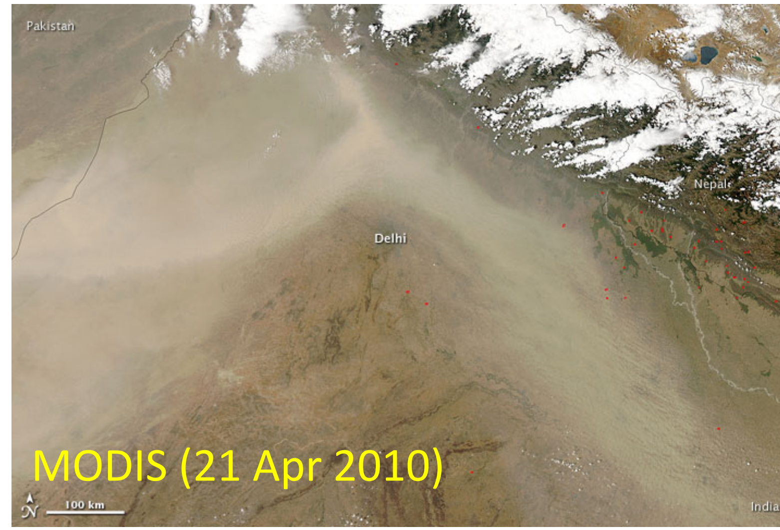
- Dry Deposition
  - Deposition velocity, vegetation (canopy or not), Henry's Law constant
  - Wesely (1989) parameterization often used
- Wet Deposition
  - Amount of cloud water, Henry's Law constant, production of precipitation, evaporation
- Henry's Law (M/atm)

  $[H_2O_2\ (aq)] = K_H\ p\_H_2O_2\ (g)$

  K_H = Henry's Law coefficient = f(temperature)

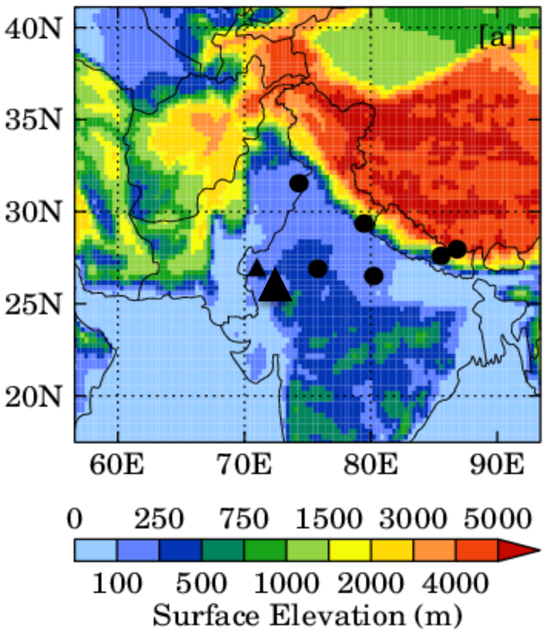
Modeling dust storm effects on aerosols and trace gases

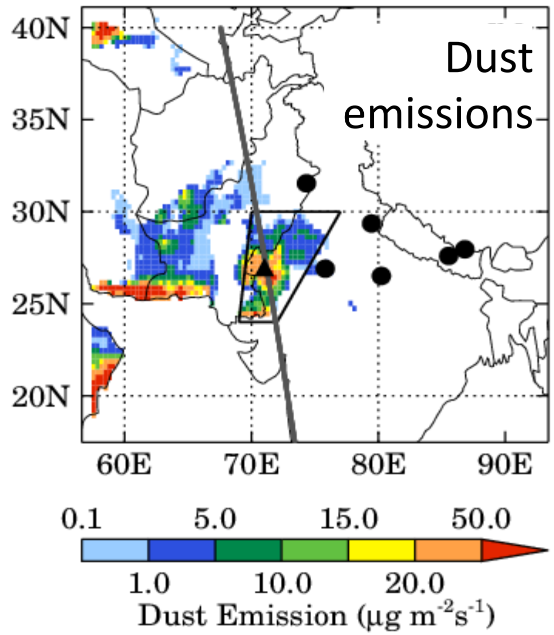


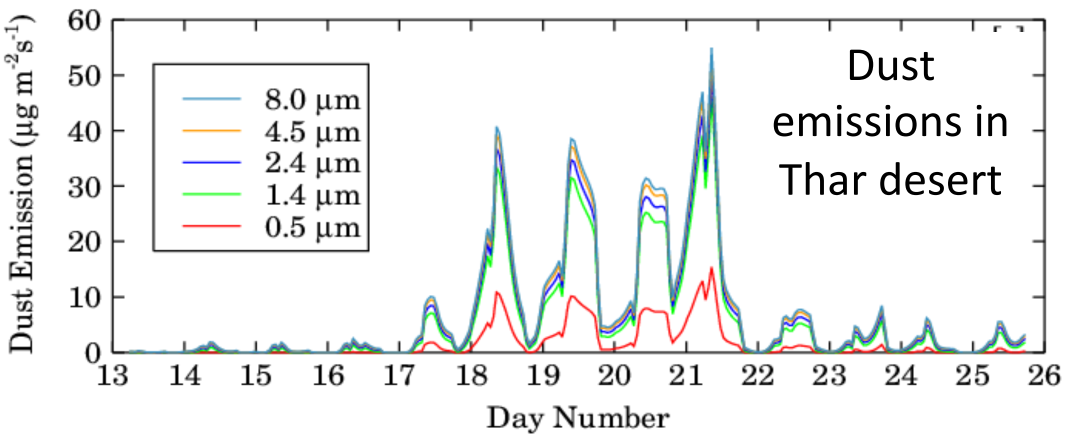


Use the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to learn what processes affect aerosols and trace gases

WRF-Chem set-up





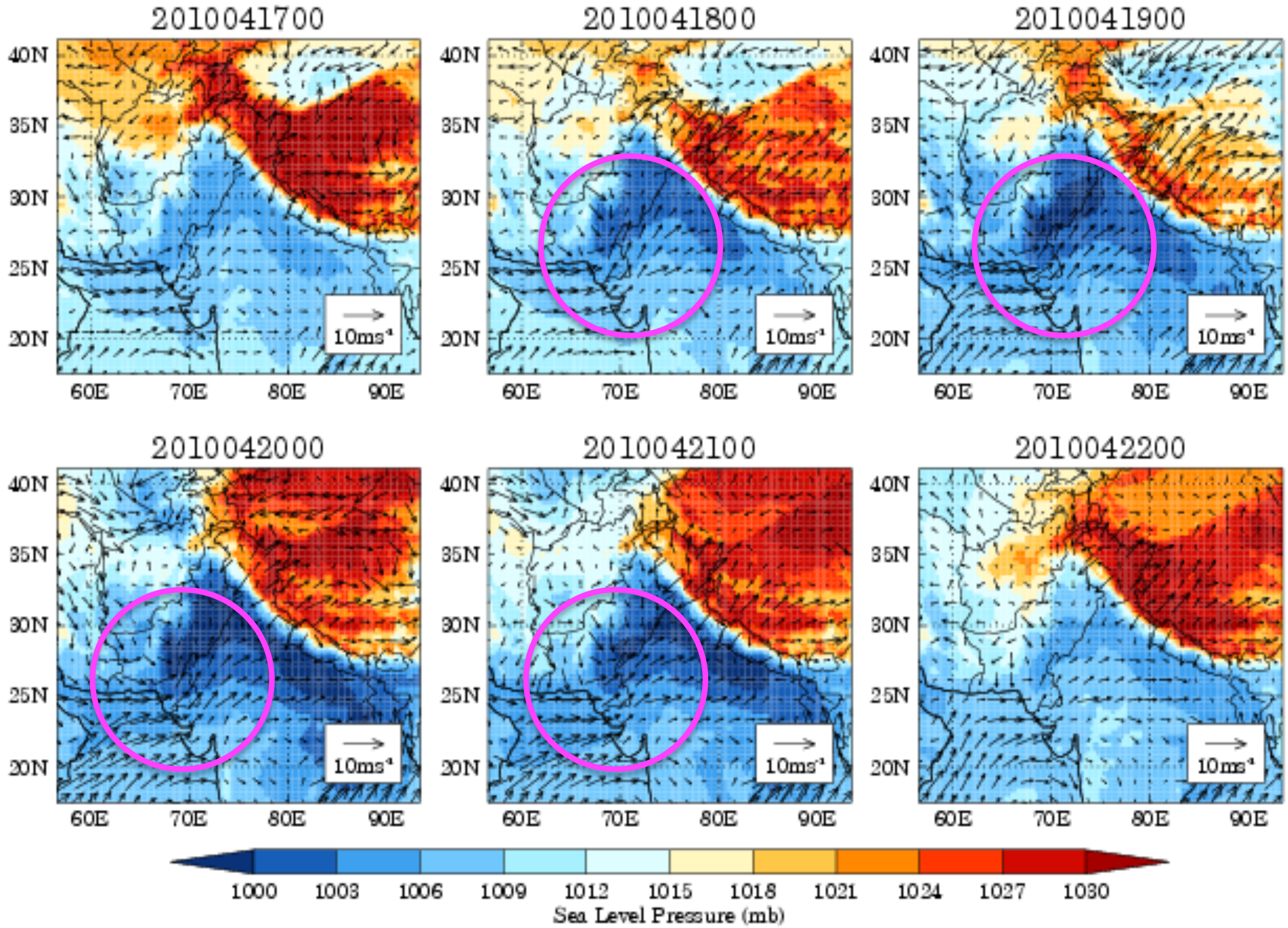


Grid spacing: 30 km
Grid points (x,y,z) = (120,90,51)
Simulation period: 10-25 Apr 2010

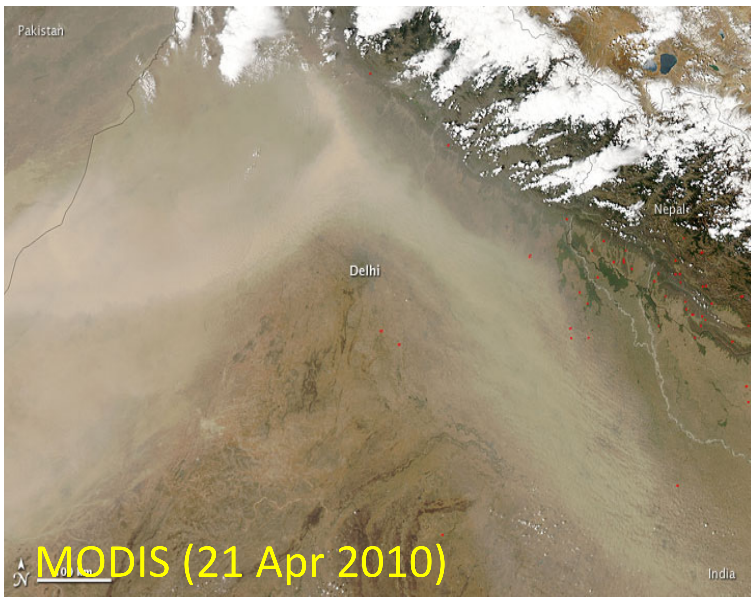
Microphysics: Thompson
Cumulus: Kain-Fritsch
Surface and PBL: MYJ Scheme
Radiation: RRTMG

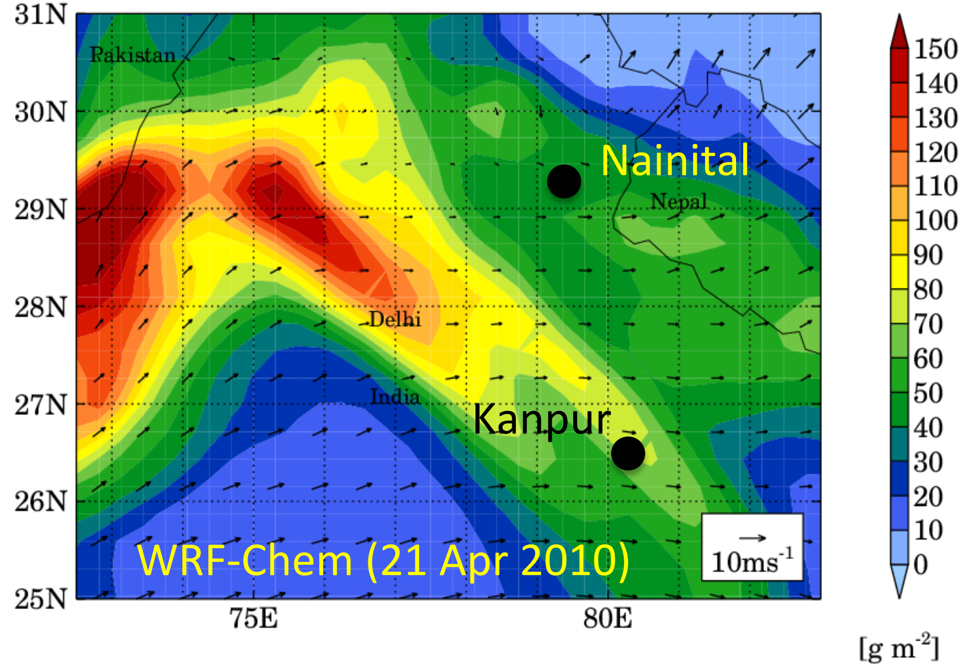
Chemical Mechanism:
  MOZART gas + GOCART aerosols
Photolysis: F-TUV
Anthro Emissions: MACCity
BB Emissions: FINN v1
Biogenic Emissions: MEGAN
Initial and Boundary Conditions:
  Meteorology: NCEP FNL
  Chemistry: MOZART-4 CTM

A low pressure region over the Thar Desert generated this dust storm.



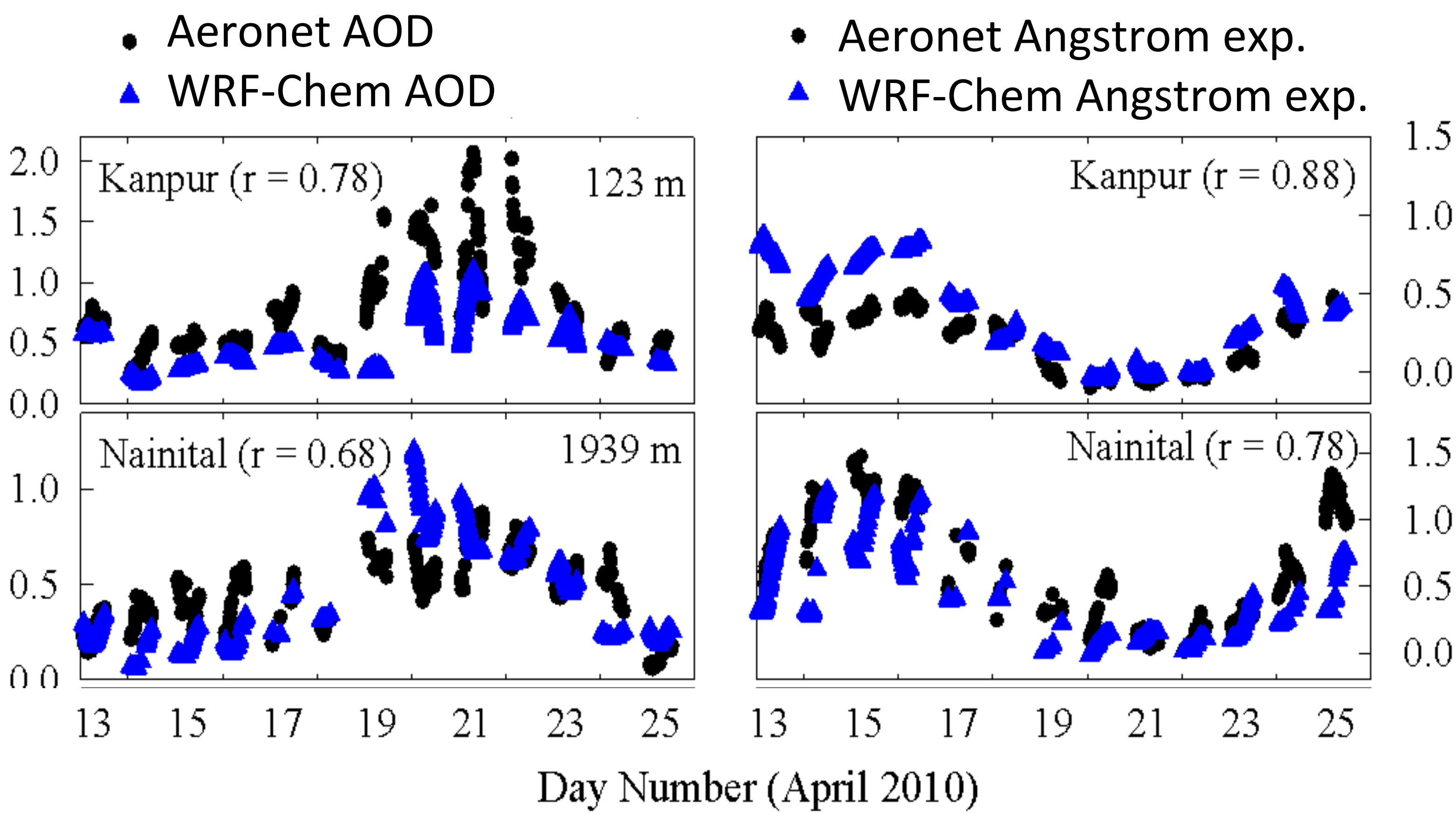
WRF-Chem captures spatial distribution of the dust storm





[Kumar et al., ACPD, 2013]

WRF-Chem captures AOD and Angstrom exponent

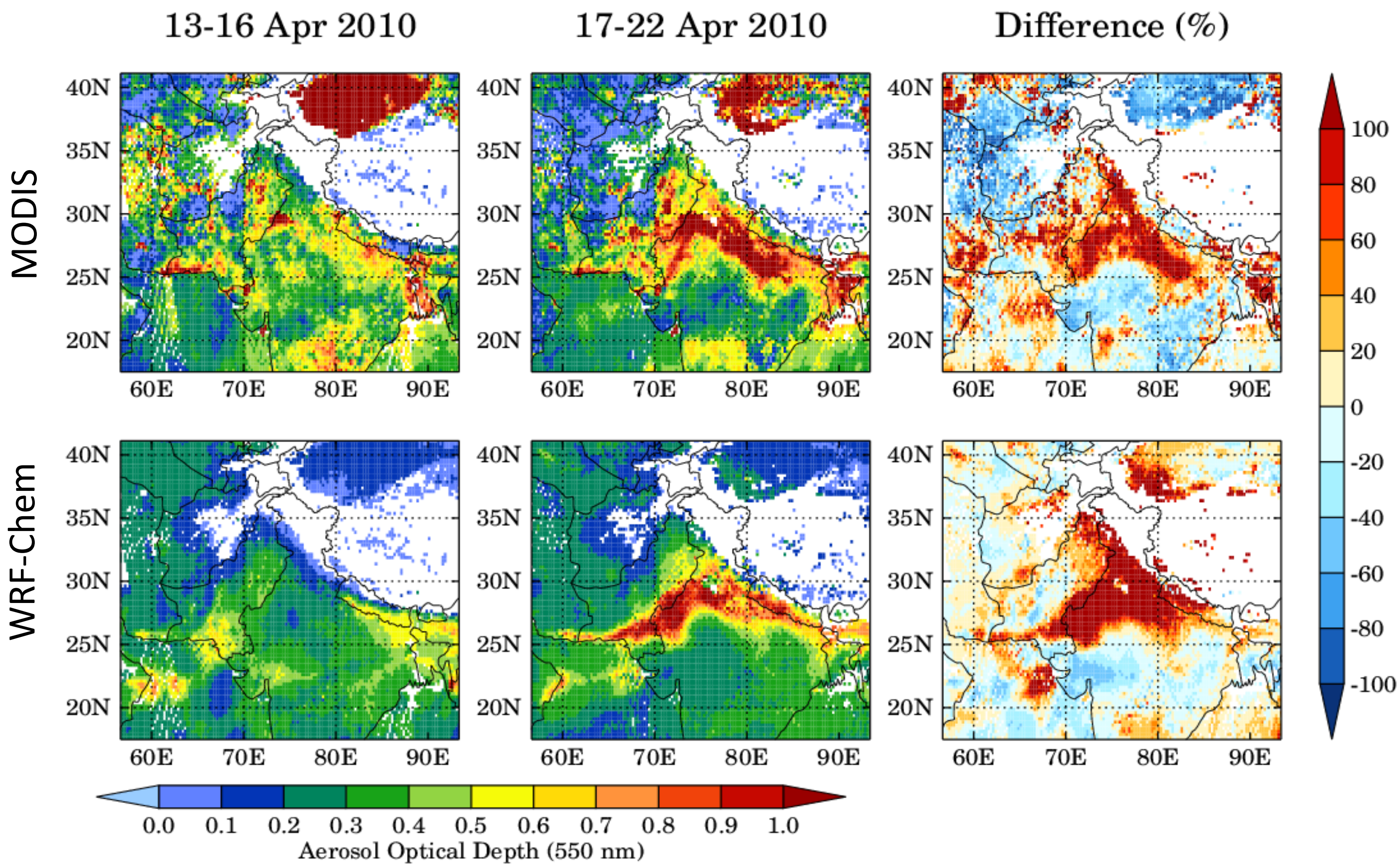


AOD – integrated extinction coefficient over a vertical column of unit cross section.

Angstrom exponent – inverse relation with aerosol size, smaller for larger aerosols and vice versa.

[Kumar et al., ACPD, 2013]

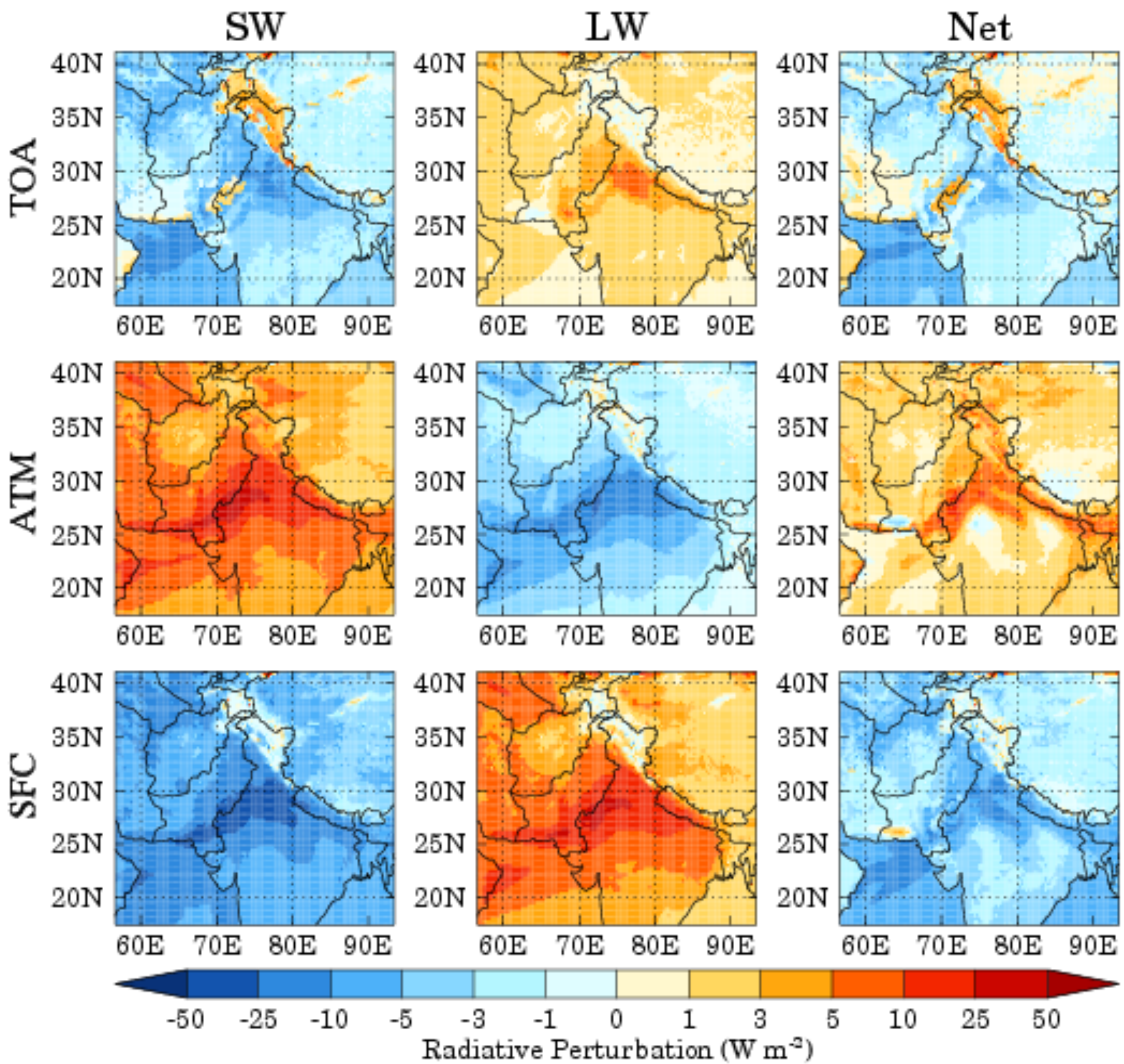
Dust Storm almost doubled the regional aerosol loading



WRF-Chem Sensitivity Simulations

1. Base Case – with Dust emissions and j-values affected = **DUST_J**
2. No Dust emissions Case = **No Dust**

Dust Storm cools the surface and TOA, and warms the atmosphere



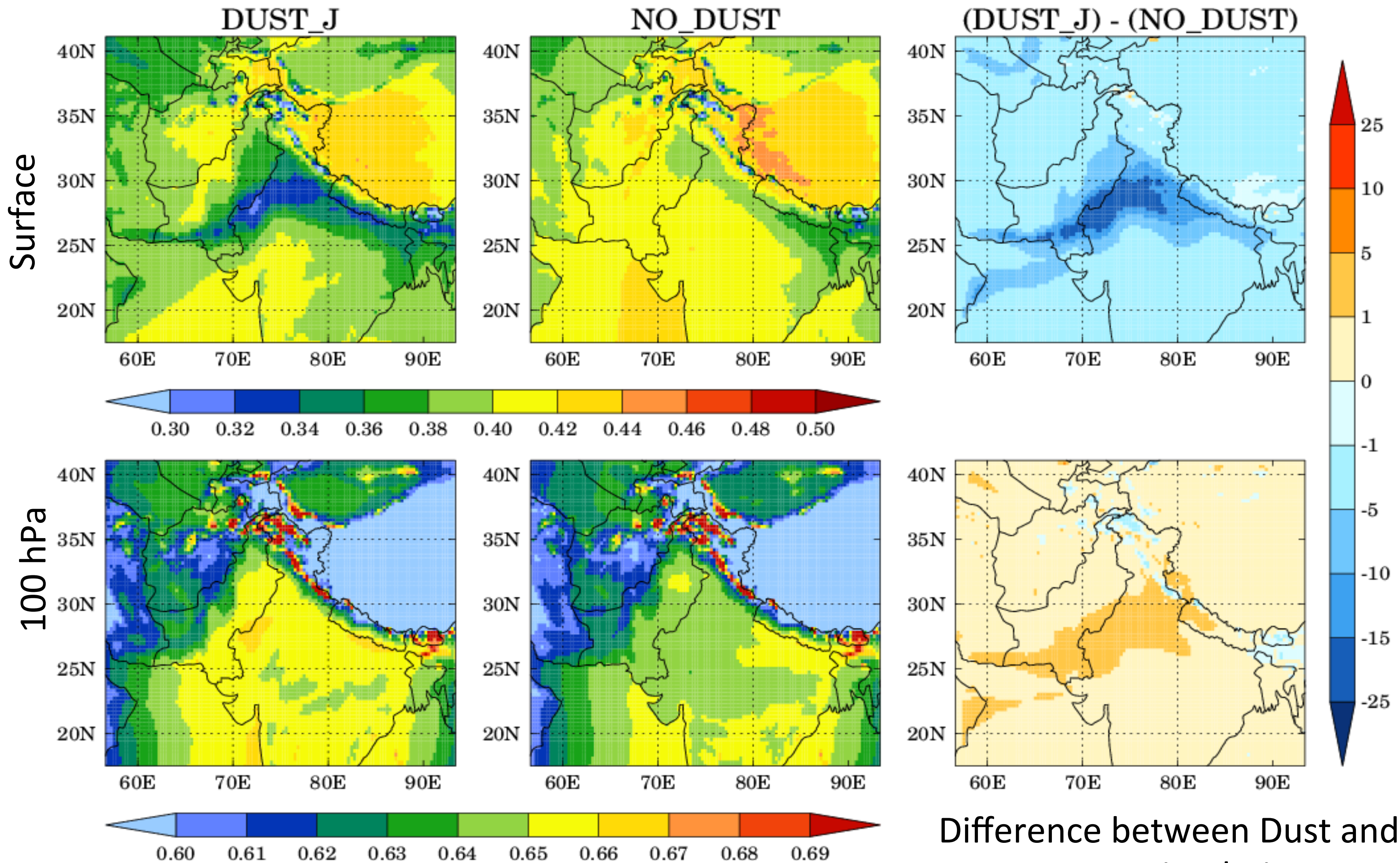
TOA

Atmosphere

Surface

Dust storm decreases photolysis rates at the surface and increases in the upper troposphere

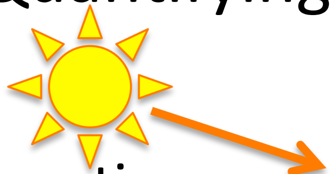
17-22 April 2010



NO_2 Photolysis Rate

Difference between Dust and No Dust simulations

Quantifying Photolysis Processes



Photolysis reaction: $NO_2 + h\nu \rightarrow NO + O$

Photolysis rates:

$$\left.\frac{d[NO_2]}{dt}\right|_{h\nu} = -j[NO_2]$$

$$\left.\frac{d[NO]}{dt}\right|_{h\nu} = \left.\frac{d[O]}{dt}\right|_{h\nu} = +j[NO_2]$$

Photolysis frequency (s^{-1}) $\quad j = \int_\lambda \sigma(\lambda)\,\phi(\lambda)\,F(\lambda)\,d\lambda$

(other names: photo-dissociation rate coefficient, J-value)

Calculation of Photolysis Coefficients

$$J\ (s^{-1}) = \int \sigma(\lambda)\, \phi(\lambda)\, F(\lambda)\, d\lambda$$

$\sigma(\lambda) =$ absorption cross section, cm^2 $molec^{-1}$

-- probability that photon is absorbed

$\phi(\lambda) =$ photodissociation quantum yield, molec $quanta^{-1}$

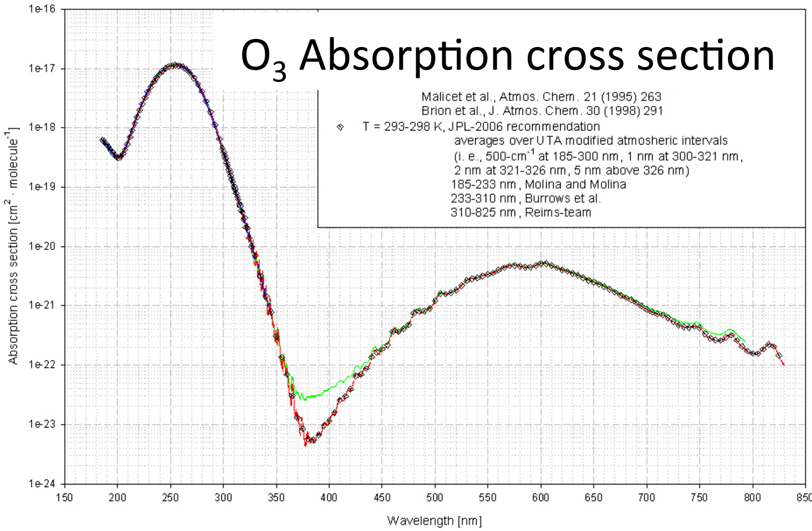
-- probability that absorbed photon causes dissociation

$F(\lambda)$ = spectral actinic flux, quanta cm^{-2} s^{-1} nm^{-1}

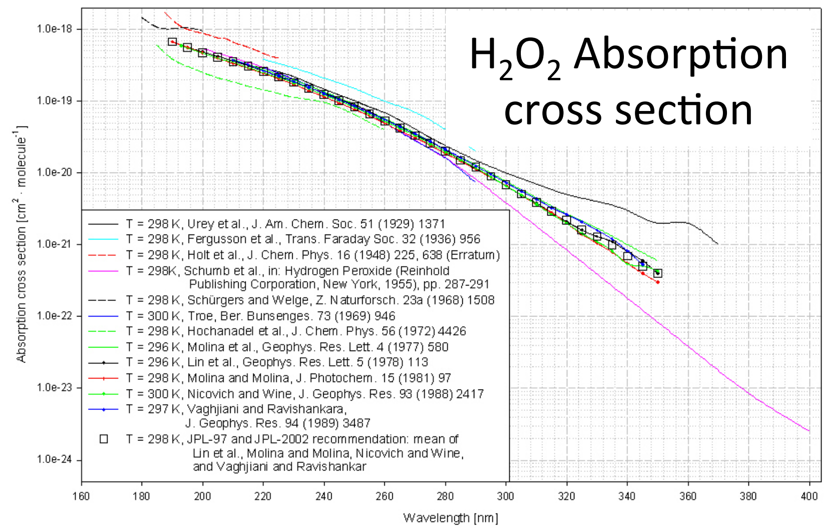
= solar radiation flux onto sphere

-- probability of photon near molecule

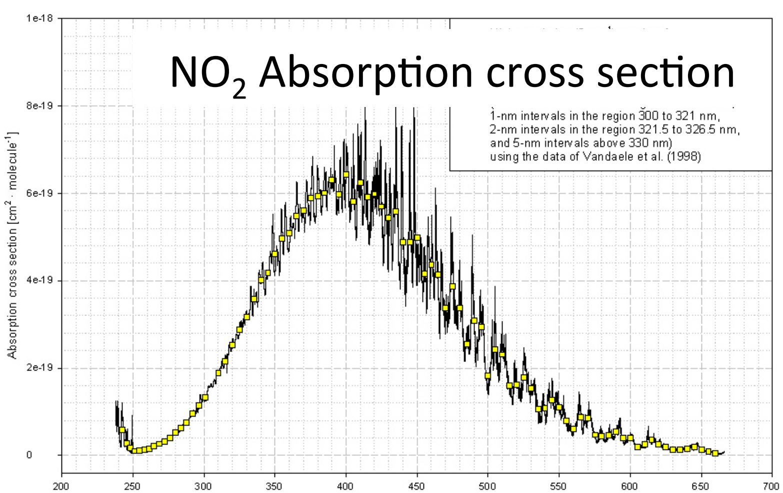
Absorption Cross Section Varies with Species and Wavelength



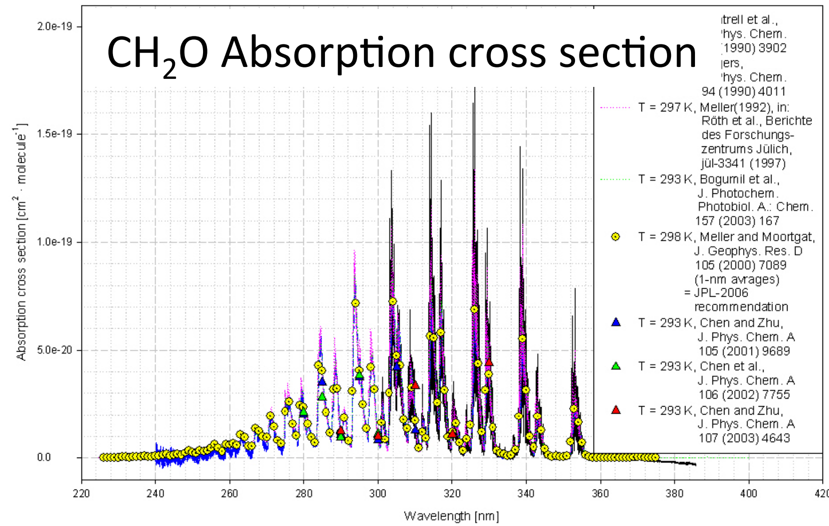
Absorption cross sections of ozone O_3 at room temperature
Evaluation for JPL-2006 recommendation



Absorption cross sections of hydrogen peroxide H_2O_2 at room temperature (180-400 nm)

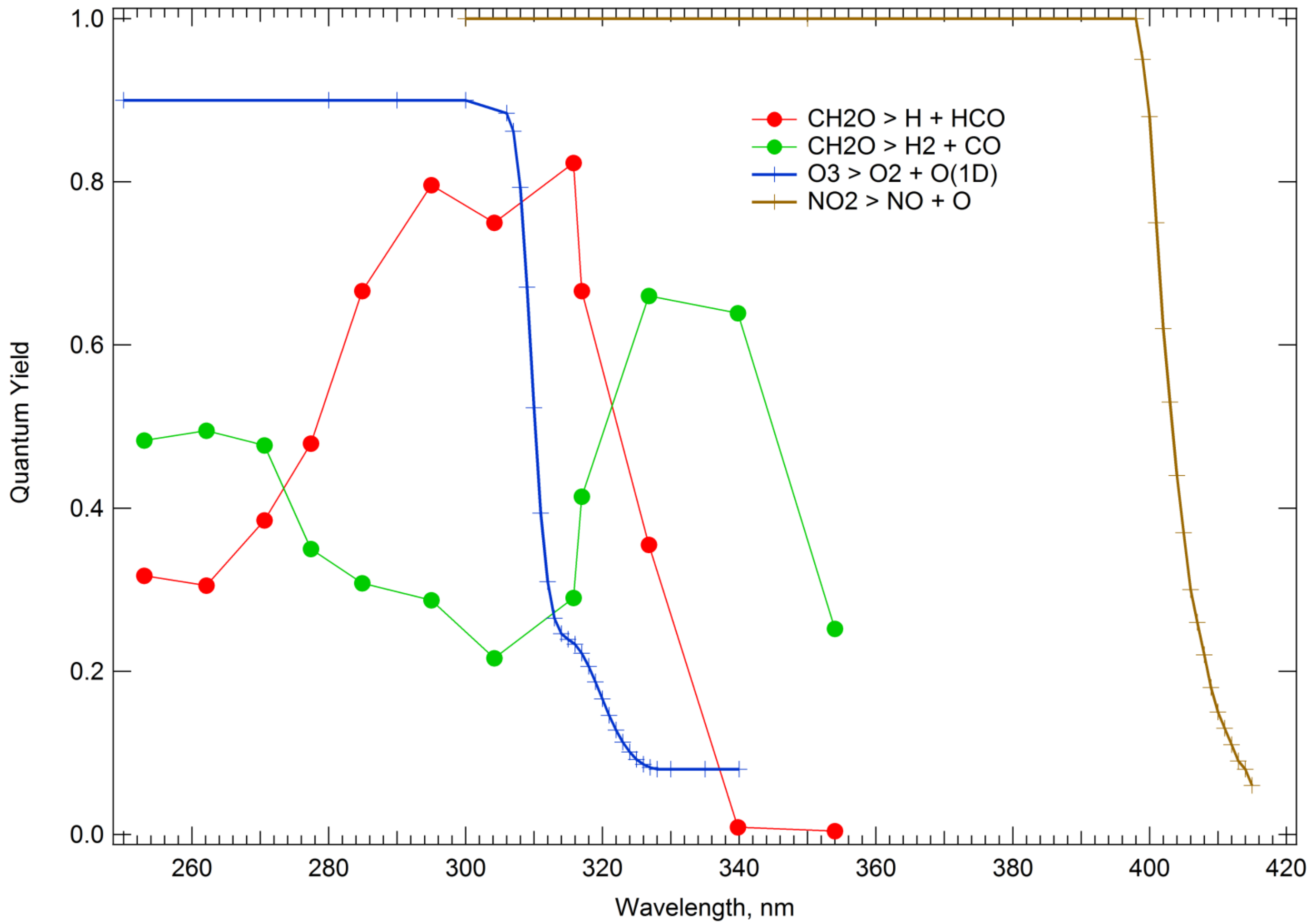


Absorption cross sections of nitrogen dioxide NO_2 at 294 K
Results from the year 1998 and JPL-2006 recommendation



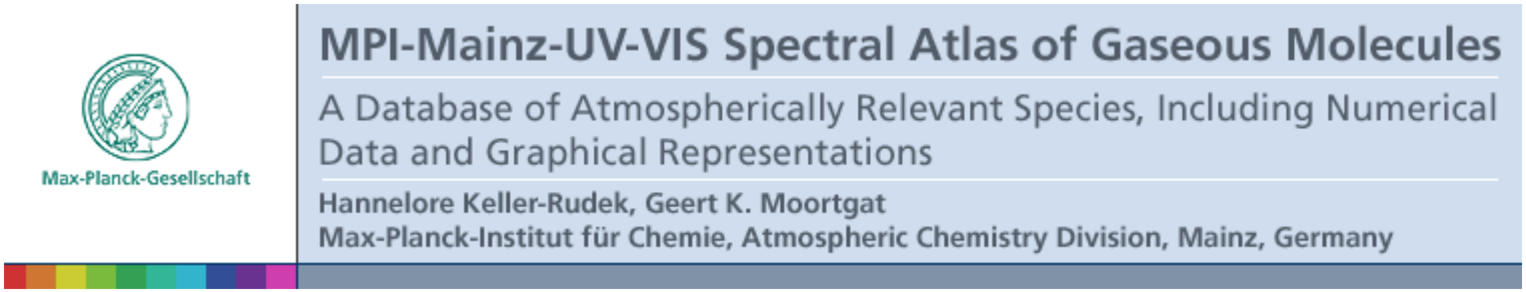
Absorption cross sections of formaldehyde CH_2O at room temperature (results 1990-2003)

Measured Quantum Yields

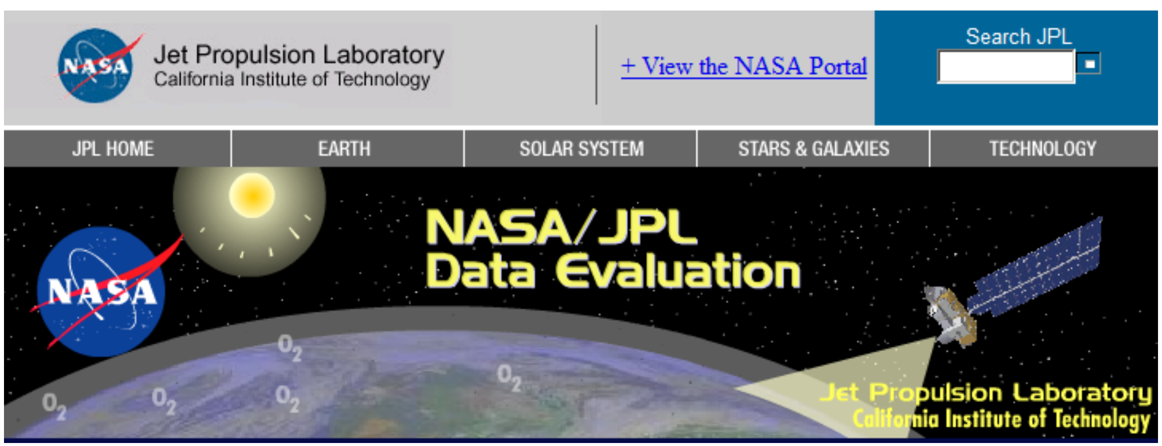


Compilations of Cross Sections & Quantum Yields

http://www.atmosphere.mpg.de/enid/2295



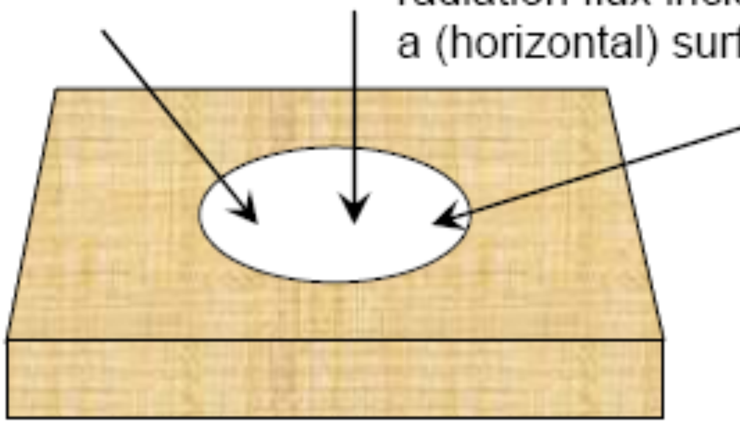
http://jpldataeval.jpl.nasa.gov/



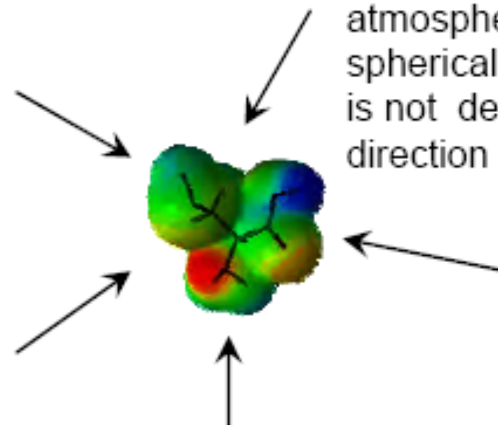
Integrals Over Angular Incidence

Irradiance vs Actinic Flux

Irradiance: The radiation flux incident on a (horizontal) surface.



Actinic flux: The photochemically active radiation flux in the earth's atmosphere. This flux is spherically integrated and is not dependent the direction of the radiation.



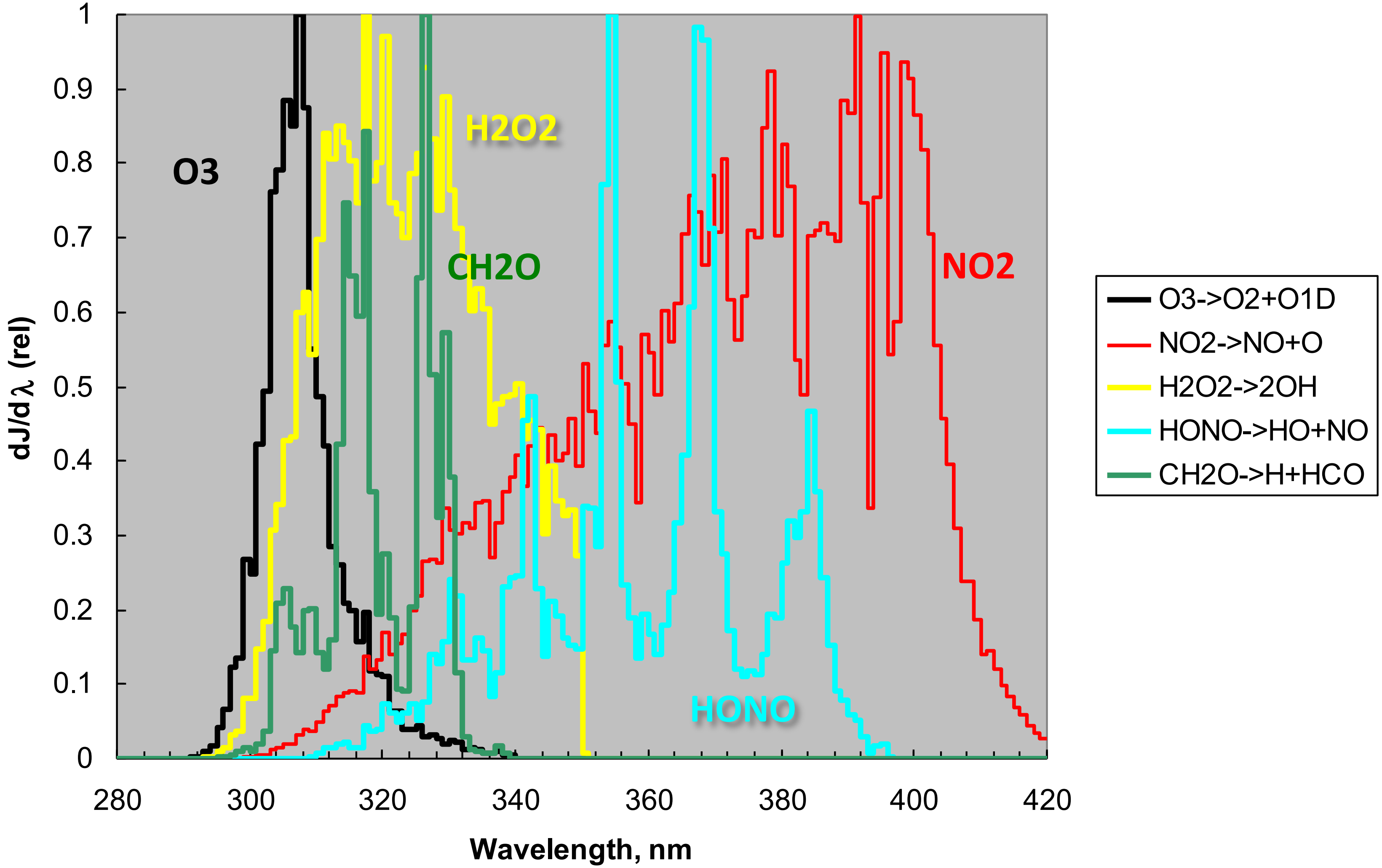
$$E = \int_0^{2\pi}\int_0^{\frac{\pi}{2}} I(\theta,\varphi)\cos\theta\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\varphi$$

Watts m^{-2}

$$F = \int_0^{\pi}\int_0^{2\pi} I(\theta,\varphi)\sin\theta\,\mathrm{d}\varphi\,\mathrm{d}\theta$$

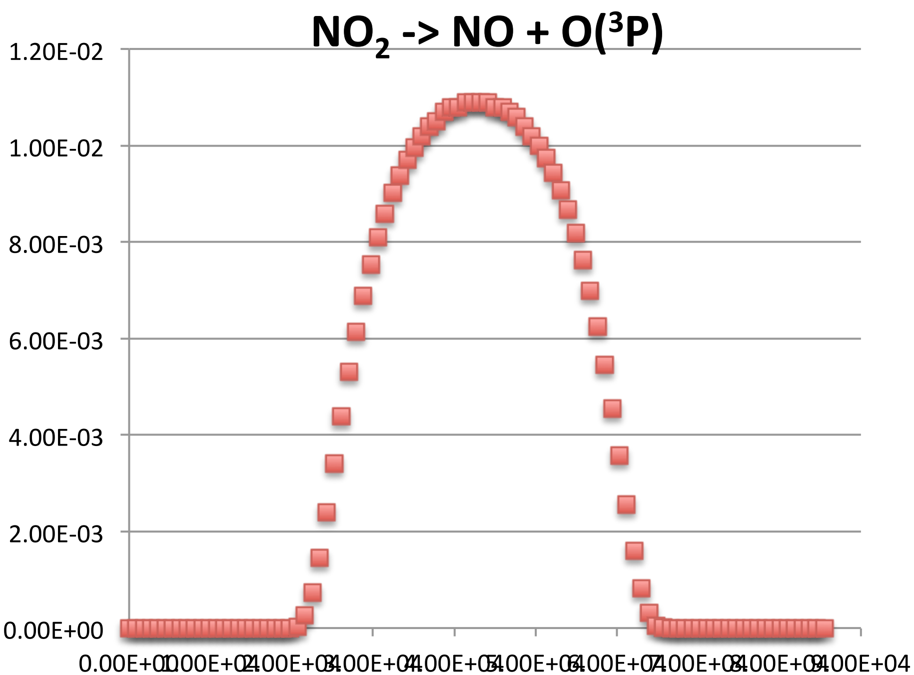
Watts m^{-2} or quanta s^{-1} cm^{-2}

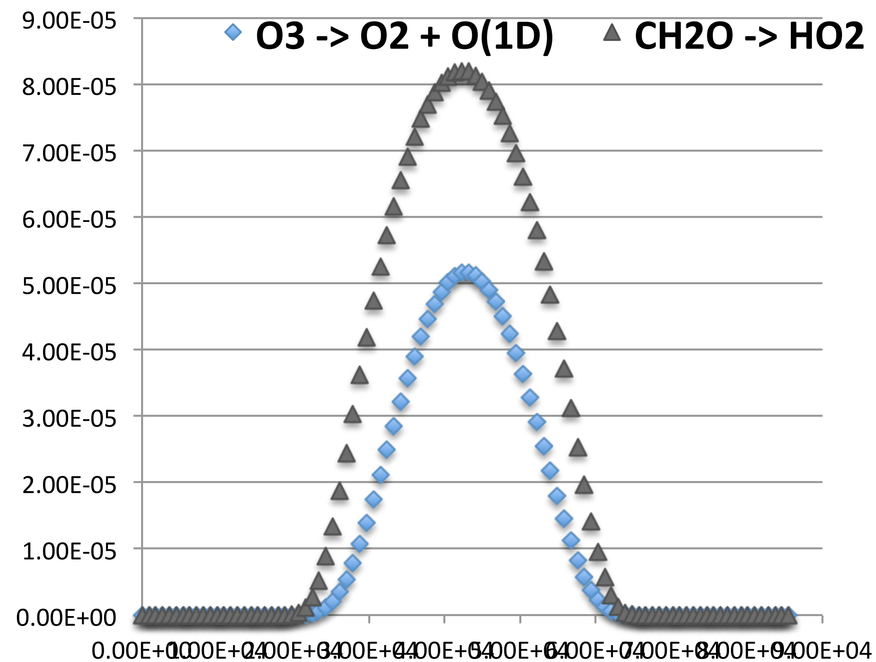
Photolysis Frequencies as Function of Wavelength



surface, overhead sun

Photolysis Frequencies and Time of Day

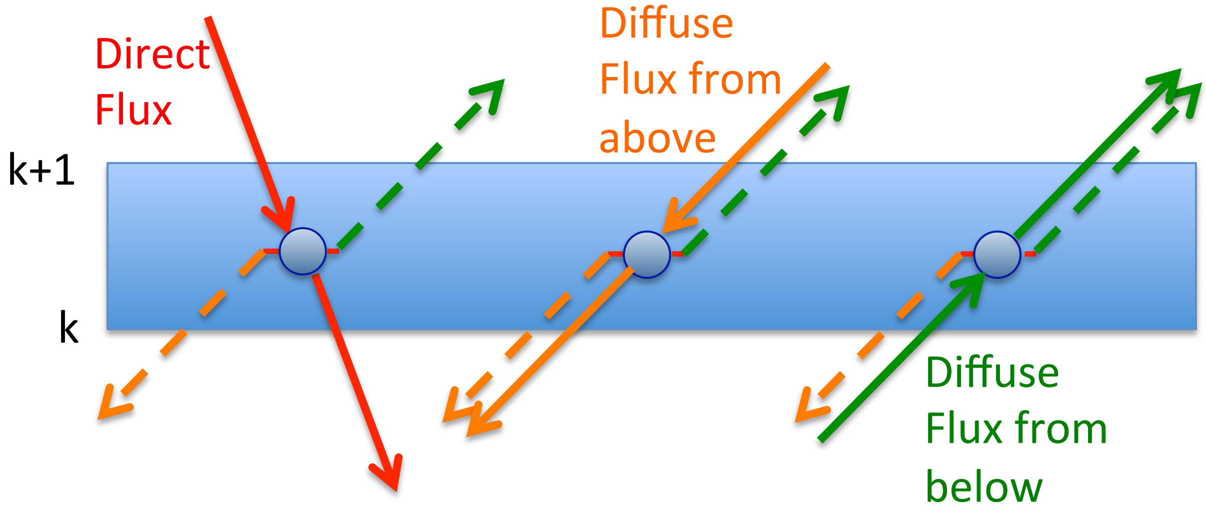




NO_2 photolysis has broader parabola
-- result of diffuse vs direct radiation

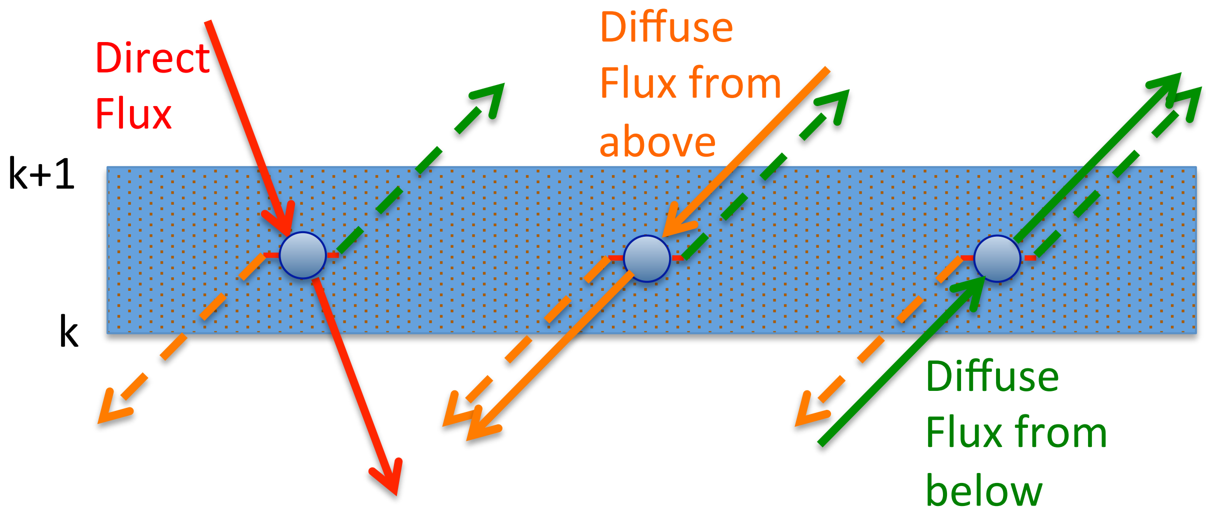
Calculating Photolysis Freqencies

Need to do Radiative Transfer Calculations



Aerosols and Clouds Affect Photolysis Rates

characteristics of the aerosol or cloud layer provides information to estimate their effect



Must specify three optical properties:

Optical depth, $\Delta\tau$

Single scattering albedo, w_o = scatt./(scatt.+abs.)

Asymmetry factor, $\mathbf{g}$: forward fraction, $f \sim (1+\mathbf{g})/2$

Vertical optical depth, $\Delta\tau(\lambda, z) = \sigma(\lambda, z)\, n(z)\, \Delta z$

for molecules: $\Delta\tau(\lambda, z) \sim 0 - 30$

Rayleigh scatt. $\sim 0.1 - 1.0$

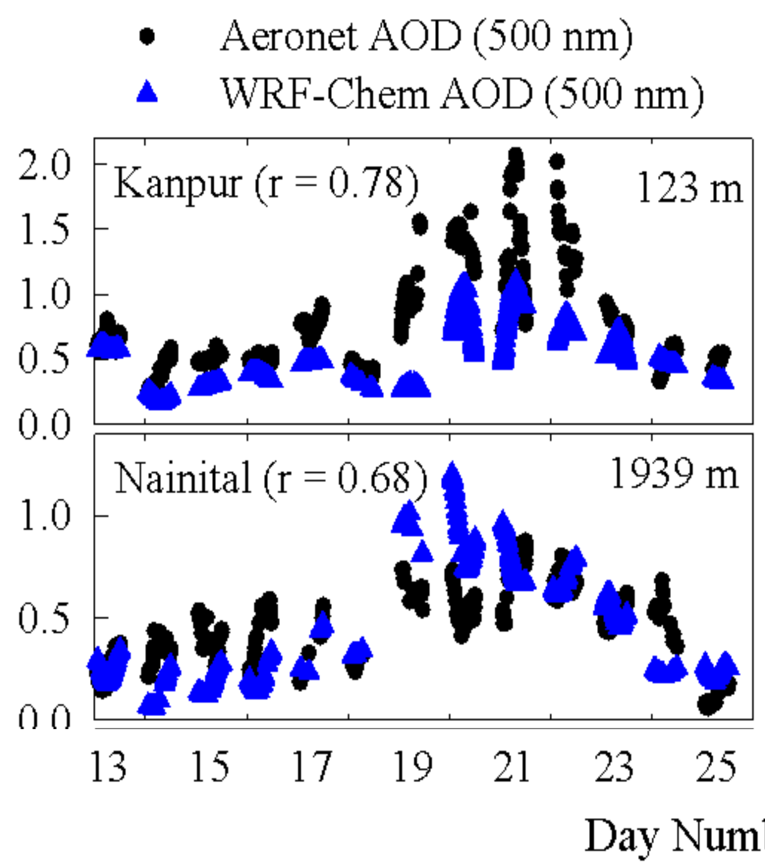
O_3 absorption $\sim 0 - 30$

for aerosols: $0.01 - 5.0$

for clouds: $1 - 1000$

cirrus $\sim 1\text{-}5$

cumulonimbus $\sim > 100$



Single Scattering Albedo

$w_o(\lambda, z)$ = scatt./(scatt.+abs.)

SSA range: 0 - 1

limits: pure scattering = 1.0

pure absorption = 0.0

for molecules, strongly λ-dependent, depending on absorber amount, esp. O_3

for aerosols:

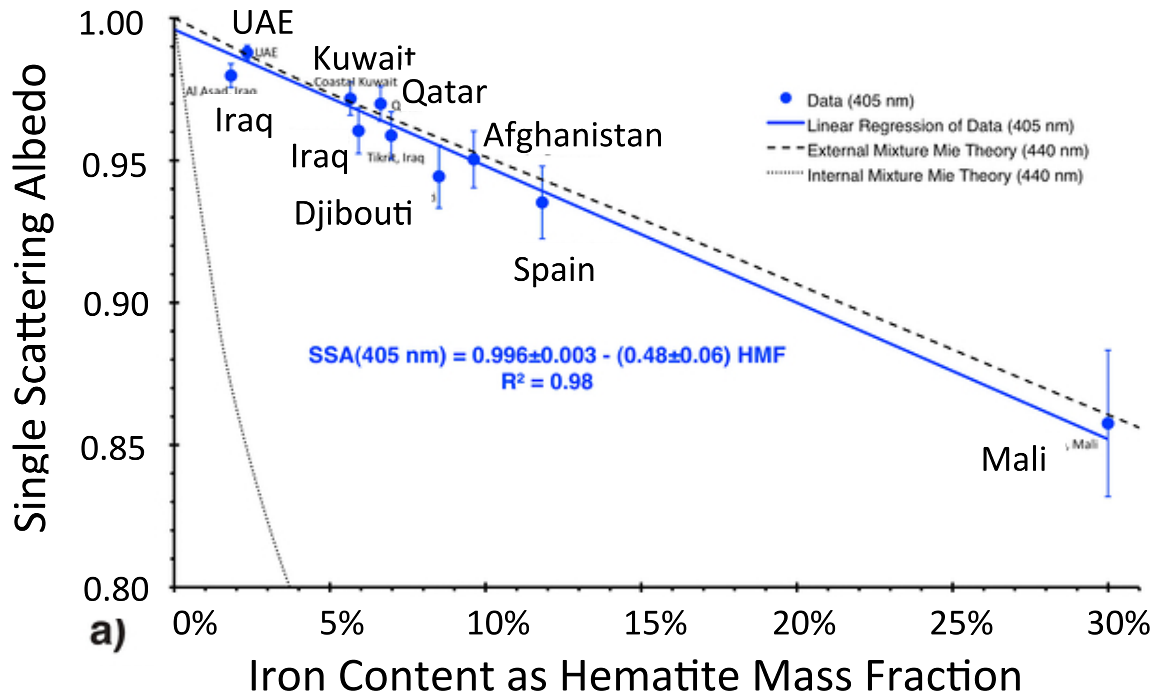
sulfate ~ 0.99

soot, organics ~ 0.8 or less,

not well known but probably higher at shorter λ, esp. in UV

for clouds: typically 0.9999 or larger (vis and UV)

Single scattering albedo of fine mineral dust aerosols controlled by iron concentration



Moosmuller et al. (2012)
Journal of Geophysical Research: Atmospheres
Volume 117, Issue D11, D11210, 8 JUN 2012 DOI: 10.1029/2011JD016909
http://onlinelibrary.wiley.com/doi/10.1029/2011JD016909/full#jgrd17711-fig-0003

Asymmetry factor, $g(\lambda, z)$

range -1 to + 1

- pure back-scattering = -1
- isotropic or Rayleigh = 0
- pure forward scattering = +1

$$g = \frac{1}{2}\int_{-1}^{+1} P(\Theta)\cos\Theta \, d(\cos\Theta)$$

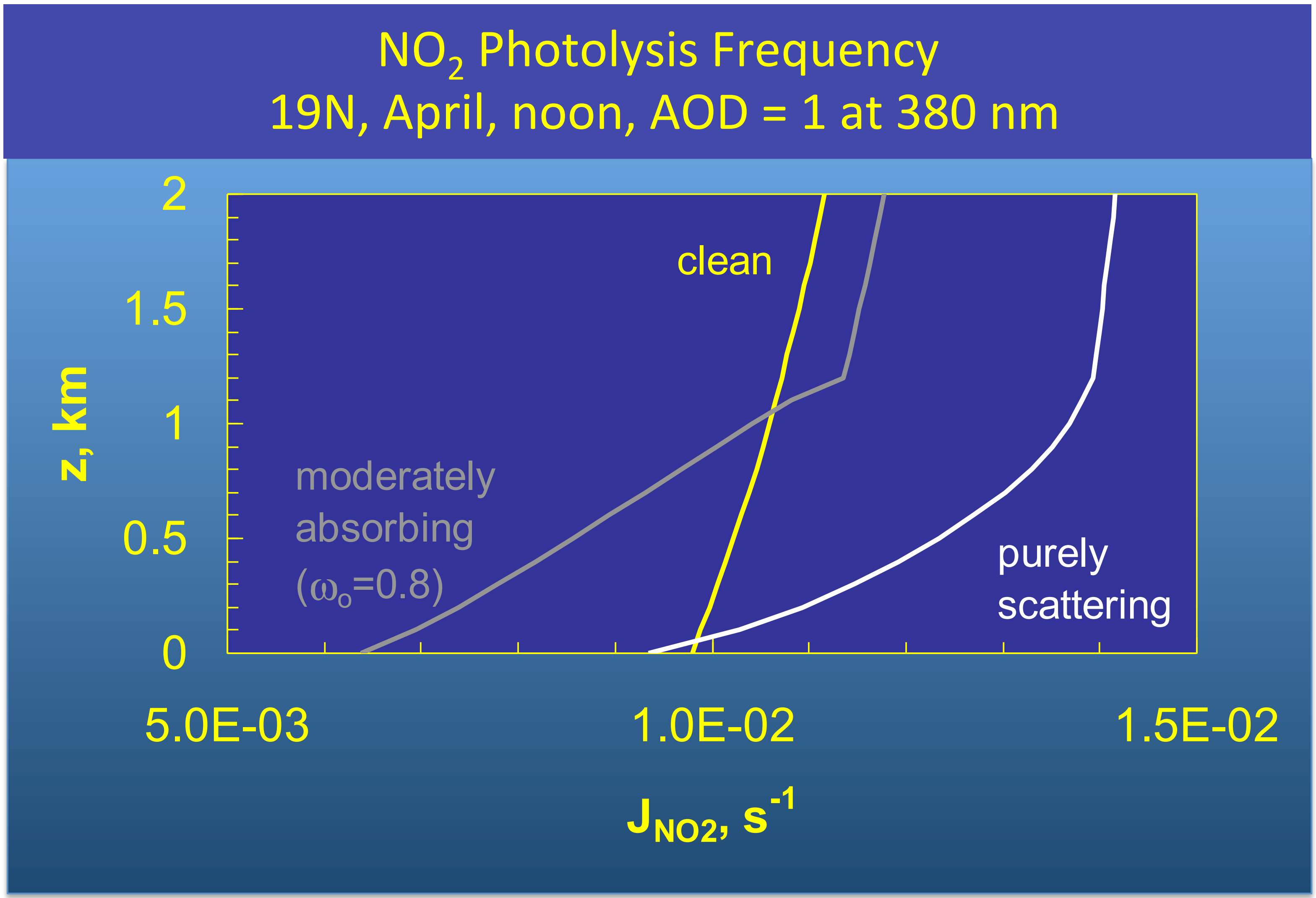
strongly dependent on particle size

- for aerosols:, typically 0.5-0.7
- for clouds, typically 0.7-0.9

Mie theory for spherical particles: can compute $\Delta\tau$, w_o, g
from knowledge of λ, particle radius and complex index of refraction

Aerosol Effects on the Radiation

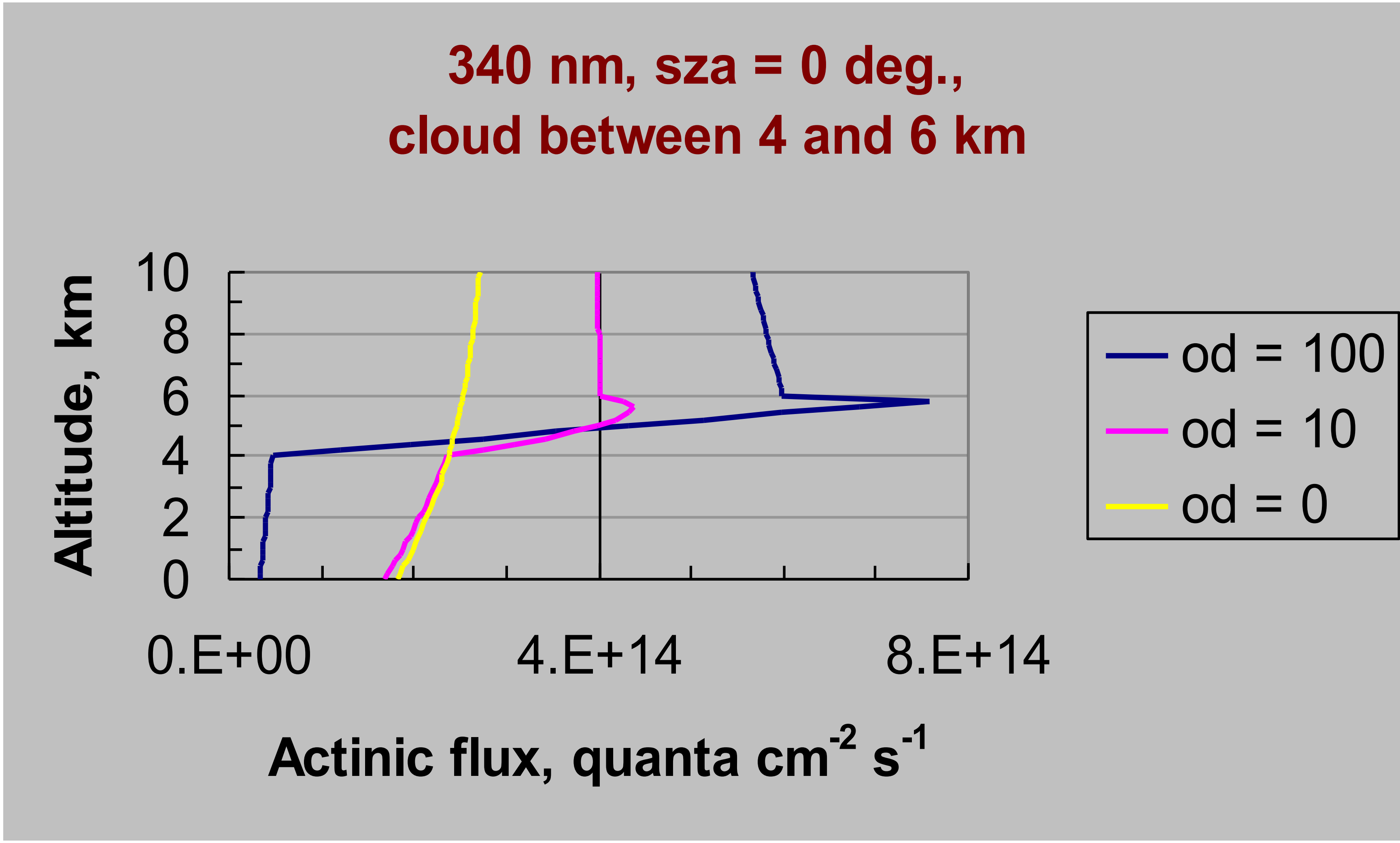
- Aerosols either scatter or absorb radiation



Uniform Cloud Layer

- Above cloud: - high radiation because of reflection
- Below cloud: - lower radiation because of attenuation by cloud
- Inside cloud: - complicated behavior
  - Top half: very high values (for high sun)
  - Bottom half: lower values

Effect Of Uniform Clouds On Actinic Flux



Numerical Solutions To Radiative Transfer Equation

- Discrete ordinates

  n-streams (n = even), angular distribution

  exact as n integrals but speed ≈ $1/n^2$
- Two-stream family

  delta-Eddington, many others

  very fast but not exact
- Monte Carlo

  slow, but ideal for 3D problems
- Others

  matrix operator, Feautrier, adding-doubling, successive orders, etc.

Irradiance calculations using SBDART: https://paulschou.com/tools/sbdart/

http://cprm.acd.ucar.edu/Models/TUV/ Photolysis Rates

cprm.acd.ucar.edu/Models/TUV/

NCAR

Chemical Processing and Regional Modeling

a research group in Atmospheric Chemistry (ACD)

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Tropospheric Ultraviolet and Visible (TUV) Radiation Model

Tropospheric ultraviolet (UV) radiation is the driving force for all tropospheric photochemical processes. Photons in the UV wavelength have the potential to break usually fairly stable molecules into very reactive fragments (photolysis) and thus initiate reaction chains otherwise unlikely or even impossible. UV radiation is also harmful to living organisms and detrimental to human health. High doses of UV radiation are considered the major contributing factor for the development of skin cancer or cataracts. UV radiation can weaken the human immune system and can affect crop yields and phytoplankton activity (to only name a few effects).

Some questions of interest might be: What factors influence the amount of UV radiation available? What is the vertical structure of the radiative field? What sort of feedbacks (e.g., increased/decreased photolysis rates) can be expected from perturbations that - directly or indirectly - affect UV radiation? What are some of the health-related effects that can be expected from changes in atmospheric composition?

Climatology of Erythemal Ultraviolet Radiation, 1979-2000

The monthly climatological distribution for the period 1979-2000 of daily total erythemal (skin-reddening) ultraviolet radiation at Earth's surface, calculated with the TUV model using satellite-based (Nimbus-7, Meteor-3 and Earth Probe) TOMS (Total Ozone Mapping Spectrometer) observations of atmospheric ozone. The effects of clouds and scattering aerosols are accounted for using TOMS reflectivity at 380 nm. Download erythemal data.

Downloads and Tools

- TUV source code
- UV Climatologies (NCAR Technical Note, figures, data)
- Quick TUV calculator

http://cprm.acd.ucar.edu/Models/TUV/ Photolysis Rates

QUICK TUV CALCULATOR

ACD > Models > TUV > Interactive_TUV

This web page runs the *4.1* version of the TUV model. You can run the model for a specified latitude, longitude and time (input option 1), or for a given solar zenith angle (input option 2). In either case, you must also specify the additional parameters in the second column. Also, you may select to print out the photolysis rates and/or the solar actinic flux spectrum at a given altitude above the surface (output option 1), or the erythemal UV and/or solar irradiance at that altitude (output option 2). For any problem, or to send comments, email TUV administrators.

INPUT OPTION 1	OTHER INPUT PARAMETERS	OUTPUT OPTION 1 (for Atmospheric Science)
LATITUDE (deg): 0	DATE (YYMMDD): 000630	☑ MOLECULAR PHOTOLYSIS FREQUENCIES (s-1)
LONGITUDE (deg): 0	OVERHEAD OZONE COLUMN (du): 300	☐ ACTINIC FLUX, SPECTRAL (quanta s-1 cm-2 nm-1)
TIME (hh:mm:ss, GMT): 12:00:00	SURFACE ALBEDO (0-1): 0.1	**OUTPUT OPTION 2 (for Biology)**
INPUT OPTION 2	GROUND ELEVATION (km asl): 0	☑ IRRADIANCE, WEIGHTED (W m-2)
SOLAR ZENITH ANGLE (deg): 0	MEASUREM. ALTITUDE (km asl): 0	☐ IRRADIANCE, SPECTRAL (W m-2 nm-1)

RADIATION TRANSFER MODEL

- (•) Pseudo-spherical 2 streams (faster, less accurate)
- ( ) Pseudo-spherical discrete ordinate 4 streams (slower, more accurate)

GO!

Photochemistry Summary

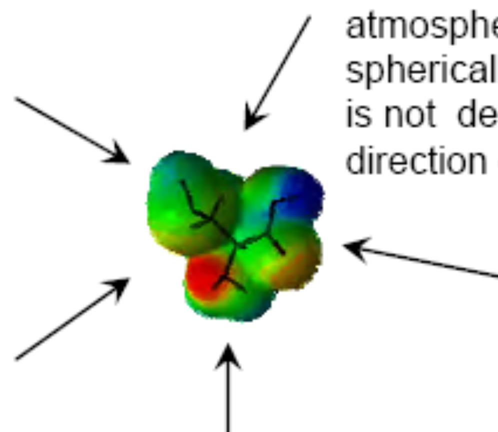
$$J\ (\mathrm{s}^{-1}) = \int \sigma(\lambda)\,\phi(\lambda)\,F(\lambda)\,d\lambda$$

$\sigma(\lambda)$ = absorption cross section, $cm^2\ molec^{-1}$

$\phi(\lambda)$ = photodissociation quantum yield, $molec\ quanta^{-1}$

$F(\lambda)$ = spectral actinic flux, $quanta\ cm^{-2}\ s^{-1}\ nm^{-1}$

- Clouds affect radiation – scattering
- Aerosols affect radiation – either scatter or absorb



Actinic flux: The photochemically active radiation flux in the earth's atmosphere. This flux is spherically integrated and is not dependent the direction of the radiation.

During Break

Go to the following web site

http://cprm.acd.ucar.edu/Models/TUV/

1) If you are able to compile and run fortran code, download the TUV code
2) Go to the TUV Quick Calculator web page

Climatology of Erythemal Ultraviolet Radiation, 1979-2000

The monthly climatological distribution for the period 1979-2000 of daily total erythemal (skin-reddening) ultraviolet radiation at Earth's surface, calculated with the TUV model using satellite-based (Nimbus-7, Meteor-3 and Earth Probe) TOMS (Total Ozone Mapping Spectrometer) observations of atmospheric ozone. The effects of clouds and scattering aerosols are accounted for using TOMS reflectivity at 380 nm. Download erythemal data.

Downloads and Tools

- TUV source code
- UV Climatologies (NCAR Technical Note, figures, data)
- Quick TUV calculator

1) Will need to create username and password; should get a zip file.

2)

http://cprm.acd.ucar.edu/Models/TUV/ Photolysis Rates

cprm.acd.ucar.edu/Models/TUV/ how to write a reference letter

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NCAR

Chemical Processing and Regional Modeling

a research group in Atmospheric Chemistry (ACD)

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Models Home | MasterMech | WRF-Chem | TUV

Tropospheric Ultraviolet and Visible (TUV) Radiation Model

Tropospheric ultraviolet (UV) radiation is the driving force for all tropospheric photochemical processes. Photons in the UV wavelength have the potential to break usually fairly stable molecules into very reactive fragments (photolysis) and thus initiate reaction chains otherwise unlikely or even impossible. UV radiation is also harmful to living organisms and detrimental to human health. High doses of UV radiation are considered the major contributing factor for the development of skin cancer or cataracts. UV radiation can weaken the human immune system and can affect crop yields and phytoplankton activity (to only name a few effects).

Some questions of interest might be: What factors influence the amount of UV radiation available? What is the vertical structure of the radiative field? What sort of feedbacks (e.g., increased/decreased photolysis rates) can be expected from perturbations that - directly or indirectly - affect UV radiation? What are some of the health-related effects that can be expected from changes in atmospheric composition?

Climatology of Erythemal Ultraviolet Radiation, 1979-2000

The monthly climatological distribution for the period 1979-2000 of daily total erythemal (skin-reddening) ultraviolet radiation at Earth's surface, calculated with the TUV model using satellite-based (Nimbus-7, Meteor-3 and Earth Probe) TOMS (Total Ozone Mapping Spectrometer) observations of atmospheric ozone. The effects of clouds and scattering aerosols are accounted for using TOMS reflectivity at 380 nm. Download erythemal data.

Downloads and Tools

- TUV source code
- UV Climatologies (NCAR Technical Note, figures, data)
- Quick TUV calculator

Quick TUV Calculator to get Photolysis Rates

QUICK TUV CALCULATOR

ACD > Models > TUV > Interactive TUV

This web page runs the *4.1* version of the TUV model. You can run the model for a specified latitude, longitude and time (input option 1), or for a given solar zenith angle (input option 2). In either case, you must also specify the additional parameters in the second column. Also, you may select to print out the photolysis rates and/or the solar actinic flux spectrum at a given altitude above the surface (output option 1), or the erythemal UV and/or solar irradiance at that altitude (output option 2). For any problem, or to send comments, email TUV administrators.

INPUT OPTION 1	OTHER INPUT PARAMETERS	OUTPUT OPTION 1 (for Atmospheric Science)
LATITUDE (deg): 0	DATE (YYMMDD): 000630	MOLECULAR PHOTOLYSIS FREQUENCIES (s-1)
LONGITUDE (deg): 0	OVERHEAD OZONE COLUMN (du): 300	ACTINIC FLUX, SPECTRAL (quanta s-1 cm-2 nm-1)
TIME (hh:mm:ss, GMT): 12:00:00	SURFACE ALBEDO (0-1): 0.1	**OUTPUT OPTION 2 (for Biology)**
INPUT OPTION 2	GROUND ELEVATION (km asl): 0	IRRADIANCE, WEIGHTED (W m-2)
SOLAR ZENITH ANGLE (deg): 0	MEASUREM. ALTITUDE (km asl): 0	IRRADIANCE, SPECTRAL (W m-2 nm-1)

RADIATION TRANSFER MODEL

- Pseudo-spherical 2 streams (faster, less accurate)
- Pseudo-spherical discrete ordinate 4 streams (slower, more accurate)

GO!

TUV Fortran Program

-- code is compiled and ready to run --

```
bodhi:~/Documents/tuv/v5.0>tuv
====================================================================
             TROPOSPHERIC ULTRAVIOLET VISIBLE (TUV) MODEL
                           (version 5.0)
          S. Madronich et al., Atmospheric Chemistry Division
               National Center for Atmospheric Research
                   P. O. Box 3000, Boulder, Colorado
                          tuv@acd.ucar.edu

                      Copyright (C) 1994-2010
             University Corporation for Atmospheric Research

====================================================================
  Type ?? for general information
  or <enter> to continue
??
```

TUV Fortran Program

-- code is compiled and ready to run --

```
??
----------------------------------------------------------------------
 The TUV model calculates solar short-wave radiation in the
 Earth's atmosphere.  Available output includes:
 -  Spectral irradiance, W m-2 nm-1
 -  Spectral actinic flux, quanta cm-2 s-1 nm-1
 -  Spectrally integrated irradiance, unweighted or weighted
      by biological action spectra, W m-2
 -  Photolysis rate coefficients, s-1
 Type ?xxx (where xxx = variable name) for help on inputs,
 e.g. type ?tmzone to get help on entering time zone.
 Inputs and outputs can be saved in different files.
 A log file (tuvlog) is also created.
   Only some simple changes are possible in the interactive
 version. Additional changes (e.g. shapes of vertical profiles
 of ozone, clouds, aerosols; wavelength dependent albedo, etc.)
 can be made by obtaining and editing the Fortran source code.
 The full TUV model is available at:
        http://www.acd.ucar.edu/TUV
----------------------------------------------------------------------
PAUSE
To resume execution, type go.  Other input will terminate the job.
```

TUV Fortran Program

-- code is compiled and ready to run --

```
go
RESUMED
================================================================
 select input file
  <enter>: usrinp (if created before)
  1: defin1 (default No. 1, optimized for surface UV)
  2: defin2 (default No. 2, optimized for photochem )
  3: defin3 (default No. 3, optimized for master mech)
  4: defin4 (default No. 4, sample of all outputs)
  file-name for others
```

defin1 → good for biology erythemal information
defin2 → gives photolysis rates of a few reactions
defin3 → gives all photolysis rates with outputs every 15 minutes for 24 hours
→ good for using as input into box model simulations

TUV Fortran Program

-- code is compiled and ready to run --

```
go
RESUMED
==================================================================
 select input file
  <enter>: usrinp (if created before)
  1: defin1 (default No. 1, optimized for surface UV)
  2: defin2 (default No. 2, optimized for photochem )
  3: defin3 (default No. 3, optimized for master mech)
  4: defin4 (default No. 4, sample of all outputs)
  file-name for others
```

defin1 → good for biology erythemal information

defin2 → gives photolysis rates of a few reactions

defin3 → gives all photolysis rates with outputs every 15 minutes for 24 hours

→ good for using as input into box model simulations

Type 2

TUV Fortran Program

Name of input file

Name of output file

Number of "streams" for radiation calc.

```
TUV inputs:
==================================================================
inpfil =        defin2   outfil =        usrout   nstr =              4
lat =            0.000   lon =            0.000   tmzone =          0.0
iyear =           2002   imonth =             3   iday =             21
zstart =         0.000   zstop =        120.000   nz =              121
wstart =       120.000   wstop =        735.000   nwint =          -156
tstart =        12.000   tstop =         20.000   nt =                5
lzenit =             F   alsurf =         0.100   psurf =        -999.0
o3col =        300.000   so2col =         0.000   no2col =        0.000
taucld =         0.000   zbase =          4.000   ztop =          5.000
tauaer =         0.235   ssaaer =         0.990   alpha =         1.000
dirsun =         1.000   difdn =          1.000   difup =         1.000
zout =           0.500   zaird =     -9.990E+02   ztemp =      -999.000
lirrad =             F   laflux =             T   lmmech =            F
lrates =             F   isfix =              0   nms =               0
ljvals =             T   ijfix =              0   nmj =               7
iwfix =              0   itfix =              0   izfix =             0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

TUV Fortran Program

Latitude

Longitude

Time Zone

```
TUV inputs:
==================================================================
inpfil =        defin2
lat =            0.000   lon =            0.000   tmzone =            0.0
iyear =           2002   imonth =             3   iday =               21
zstart =         0.000   zstop =        120.000   nz =                121
wstart =       120.000   wstop =        735.000   nwint =            -156
tstart =        12.000   tstop =         20.000   nt =                  5
lzenit =             F   alsurf =         0.100   psurf =          -999.0
o3col =        300.000   so2col =         0.000   no2col =          0.000
taucld =         0.000   zbase =          4.000   ztop =            5.000
tauaer =         0.235   ssaaer =         0.990   alpha =           1.000
dirsun =         1.000   difdn =          1.000   difup =           1.000
zout =           0.500   zaird =     -9.990E+02   ztemp =        -999.000
lirrad =             F   laflux =             T   lmmech =              F
lrates =             F   isfix =              0   nms =                 0
ljvals =             T   ijfix =              0   nmj =                 7
iwfix =              0   itfix =              0   izfix =               0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

TUV Fortran Program

Year

Month

Day

```
TUV inputs:
==================================================================
inpfil =       defin2
lat =           0.000
iyear =          2002   imonth =              3   iday =              21
zstart =        0.000   zstop =         120.000   nz =               121
wstart =      120.000   wstop =         735.000   nwint =           -156
tstart =       12.000   tstop =          20.000   nt =                 5
lzenit =            F   alsurf =          0.100   psurf =         -999.0
o3col =       300.000   so2col =          0.000   no2col =         0.000
taucld =        0.000   zbase =           4.000   ztop =           5.000
tauaer =        0.235   ssaaer =          0.990   alpha =          1.000
dirsun =        1.000   difdn =           1.000   difup =          1.000
zout =          0.500   zaird =      -9.990E+02   ztemp =       -999.000
lirrad =            F   laflux =              T   lmmech =             F
lrates =            F   isfix =               0   nms =                0
ljvals =            T   ijfix =               0   nmj =                7
iwfix =             0   itfix =               0   izfix =              0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

TUV Fortran Program

```
TUV inputs:
==========================================================================
inpfil =        defin2   outfil =         usrout
lat =            0.000   l...                0.000
iyear =           2002
zstart =         0.000   zstop =         120.000   nz =               121
wstart =       120.000   wstop =         735.000   nwint =           -156
tstart =        12.000   tstop =          20.000   nt =                 5
lzenit =             F   alsurf =          0.100   psurf =         -999.0
o3col =        300.000   so2col =          0.000   no2col =         0.000
taucld =         0.000   zbase =           4.000   ztop =           5.000
tauaer =         0.235   ssaaer =          0.990   alpha =          1.000
dirsun =         1.000   difdn =           1.000   difup =          1.000
zout =           0.500   zaird =      -9.990E+02   ztemp =       -999.000
lirrad =             F   laflux =              T   lmmech =             F
lrates =             F   isfix =               0   nms =                0
ljvals =             T   ijfix =               0   nmj =                7
iwfix =              0   itfix =               0   izfix =              0
==========================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Surface elevation above sea level

Top of atmosphere

Number of vertical levels

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =       defin2  outfil =       usrout  nstr =            4
lat =           0.000  lon =           0.000
iyear =          2002
zstart =        0.000
wstart =      120.000  wstop =       735.000  nwint =        -156
tstart =       12.000  tstop =        20.000
lzenit =            F  alsurf =        0.100
o3col =       300.000  so2col =        0.000
taucld =        0.000  zbase =         4.000
tauaer =        0.235  ssaaer =        0.990  alpha =         1.000
dirsun =        1.000  difdn =         1.000  difup =         1.000
zout =          0.500  zaird =    -9.990E+02  ztemp =      -999.000
lirrad =            F  laflux =            T  lmmech =            F
lrates =            F  isfix =             0  nms =               0
ljvals =            T  ijfix =             0  nmj =               7
iwfix =             0  itfix =             0  izfix =             0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Starting wavelength

Last wavelength

Number of wavelength intervals

If nwint < 0, the standard atmosphere wavelength grid is used

TUV Fortran Program

```
TUV inputs:
==========================================================================
inpfil =      defin2   outfil =      usrout   nstr =             4
lat =          0.000   lon =          0.000   tmzone =         0.0
iyear =         2002   imonth =           3   iday =            21
zstart =       0.000
wstart =     120.000
tstart =      12.000   tstop =       20.000   nt =               5
lzenit =           F   alsurf =       0.100   psurf =       -999.0
o3col =      300.000   so2col =       0.000   no2col =       0.000
taucld =       0.000   zbase =        4.000   ztop =         5.000
tauaer =       0.235   ssaaer =       0.990   alpha =        1.000
dirsun =       1.000   difdn =        1.000   difup =        1.000
zout =         0.500   zaird =   -9.990E+02   ztemp =     -999.000
lirrad =           F   laflux =           T   lmmech =           F
lrates =           F   isfix =            0   nms =              0
ljvals =           T   ijfix =            0   nmj =              7
iwfix =            0   itfix =            0   izfix =            0
==========================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Starting time, local hours

Stopping time

Number of time steps

TUV Fortran Program

False = use time
True = use solar zenith angle

Surface albedo

Surface pressure

If psurf < 0, then use US Standard Atmosphere (1976)

```
TUV inputs:
==================================================================
inpfil =      defin2   outfil =      usrout   nstr =           4
lat =          0.000   lon =          0.000   tmzone =       0.0
iyear =         2002   imonth =           3   iday =          21
zstart =       0.000   zstop =      120.000   nz =           121
wstart =     120.000
tstart =      12.000
lzenit =           F   alsurf =       0.100   psurf =     -999.0
o3col =      300.000   so2col =       0.000   no2col =     0.000
taucld =       0.000   zbase =        4.000
tauaer =       0.235   ssaaer =       0.990
dirsun =       1.000   difdn =        1.000
zout =         0.500   zaird =   -9.990E+02   ztemp =   -999.000
lirrad =           F   laflux =           T   lmmech =         F
lrates =           F   isfix =            0   nms =            0
ljvals =           T   ijfix =            0   nmj =            7
iwfix =            0   itfix =            0   izfix =          0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =      defin2   outfil =      usrout   nstr =           4
lat =          0.000   lon =          0.000   tmzone =       0.0
iyear =         2002   imonth =           3   iday =          21
zstart =       0.000   zstop =      120.000   nz =           121
wstart =     120.000   wstop =      735.000   nwint =       -156
tstart =      12.000
lzenit =           F
o3col =      300.000   so2col =       0.000   no2col =     0.000
taucld =       0.000   zbase =        4.000   ztop =       5.000
tauaer =       0.235   ssaaer =       0.990   alpha =      1.000
dirsun =       1.000   difdn =        1.000   difup =      1.000
zout =         0.500   zaird =   -9.990E+02   ztemp =   -999.000
lirrad =           F   laflux =           T   lmmech =         F
lrates =           F   isfix =            0   nms =            0
ljvals =           T   ijfix =            0   nmj =            7
iwfix =            0   itfix =            0   izfix =          0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Ozone column (DU)

SO_2 column (DU)

NO_2 column (DU)

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =        defin2  outfil =        usrout  nstr =          4
lat =            0.000  lon =            0.000  tmzone =      0.0
iyear =           2002  imonth =             3  iday =         21
zstart =         0.000  zstop =        120.000  nz =          121
wstart =       120.000  wstop =        735.000  nwint =      -156
tstart =        12.000  tstop =         20.000  nt =            5
lzenit =             F
o3col =        300.000
taucld =         0.000  zbase =          4.000  ztop =      5.000
tauaer =         0.235  ssaaer =         0.990  alpha =     1.000
dirsun =         1.000  difdn =          1.000  difup =     1.000
zout =           0.500  zaird =     -9.990E+02  ztemp =  -999.000
lirrad =             F  laflux =             T  lmmech =        F
lrates =             F  isfix =              0  nms =           0
ljvals =             T  ijfix =              0  nmj =           7
iwfix =              0  itfix =              0  izfix =         0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Cloud Optical Depth

Cloud base height

Cloud top height (km)

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =      defin2  outfil =      usrout  nstr =              4
lat =          0.000  lon =          0.000  tmzone =          0.0
iyear =         2002  imonth =           3  iday =             21
zstart =       0.000  zstop =      120.000  nz =              121
wstart =     120.000  wstop =      735.000  nwint =          -156
tstart =      12.000  tstop =       20.000  nt =                5
lzenit =           F                        psurf =        -999.0
o3col =      300.000
taucld =       0.000
tauaer =       0.235  ssaaer =       0.990  alpha =         1.000
dirsun =       1.000  difdn =        1.000  difup =         1.000
zout =         0.500  zaird =   -9.990E+02  ztemp =      -999.000
lirrad =           F  laflux =           T  lmmech =            F
lrates =           F  isfix =            0  nms =               0
ljvals =           T  ijfix =            0  nmj =               7
iwfix =            0  itfix =            0  izfix =             0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Aerosol Optical Depth

Single Scattering Albedo of Aerosol

Angstrom Coef.

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =       defin2   outfil =       usrout   nstr =            4
lat =           0.000   lon =           0.000   tmzone =        0.0
iyear =          2002   imonth =            3   iday =           21
zstart =        0.000   zstop =       120.000   nz =            121
wstart =      120.000   wstop =       735.000   nwint =        -156
tstart =       12.000   tstop =        20.000   nt =              5
lzenit =            F   alsurf =        0.100   psurf =      -999.0
o3col =       300.000                           no2col =      0.000
taucld =        0.000
tauaer =        0.235
dirsun =        1.000   difdn =         1.000   difup =       1.000
zout =          0.500   zaird =    -9.990E+02   ztemp =    -999.000
<enter> = keep these settings, or
Type variable name to change (lower case):
```

Direct Sun Radiation

Diffuse Down Radiation

Diffuse Up Radiation

dirsun = difdn = 1.0, difup = 0 for total down-welling irradiance
dirsun = difdn = difup = 1.0 for actinic flux from all directions
dirsun = difdn = 1.0, difup = -1 for net irradiance

These numbers are different in each of the defin# files

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =       defin2   outfil =       usrout   nstr =           4
lat =           0.000   lon =           0.000   tmzone =       0.0
iyear =          2002   imonth =            3   iday =          21
zstart =        0.000   zstop =       120.000   nz =           121
wstart =      120.000   wstop =       735.000   nwint =       -156
tstart =       12.000   tstop =        20.000   nt =             5
lzenit =            F   alsurf =        0.100   psurf =     -999.0
o3col =       300.000                           no2col =     0.000
taucld =        0.000
tauaer =        0.235
dirsun =        1.000
zout =          0.500   zaird =    -9.990E+02   ztemp =   -999.000
lirrad =            F   laflux =            T   lmmech =         F
lrates =            F
ljvals =            T
iwfix =             0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Altitude (km) for desired output

Air density (molec cm^{-3}) of output altitude

Temperature (K) of output altitude

If zaird or ztemp < 0, then US Standard Atmosphere at zout is used

TUV Fortran Program

```
TUV inputs:
==================================================================================
inpfil =       defin2   outfil =       usrout   nstr =            4
lat =           0.000   lon =           0.000   tmzone =        0.0
iyear =          2002   imonth =            3   iday =           21
zstart =        0.000   zstop =       120.000   nz =            121
wstart =      120.000   wstop =       735.000   nwint =        -156
tstart =       12.000   tstop =        20.000   nt =              5
lzenit =            F   alsurf =        0.100   psurf =      -999.0
o3col =       300.000   so2col =        0.000   no2col =      0.000
taucld =        0.000   zbase =         4.000   ztop =        5.000
tauaer =        0.235
dirsun =        1.000
zout =          0.500
lirrad =            F   laflux =            T   lmmech =          F
lrates =            F   isfix =             0   nms =             0
ljvals =            T   ijfix =             0   nmj =             7
iwfix =             0   itfix =             0   izfix =           0
==================================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Output includes actinic flux

Output includes data for box model

True or False for whether spectral irradiance is included in output

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =      defin2   outfil =        usrout   nstr =            4
lat =          0.000   lon =            0.000   tmzone =        0.0
iyear =         2002   imonth =             3   iday =           21
zstart =       0.000   zstop =        120.000   nz =            121
wstart =     120.000   wstop =        735.000   nwint =        -156
tstart =      12.000   tstop =         20.000   nt =              5
lzenit =           F   alsurf =         0.100   psurf =      -999.0
o3col =      300.000   so2col =         0.000   no2col =      0.000
taucld =       0.000                            ztop =        5.000
tauaer =       0.235                            alpha =       1.000
dirsun =       1.000
zout =         0.500
lirrad =           F
lrates =           F   isfix =              0   nms =             0
ljvals =           T   ijfix =              0   nmj =             7
iwfix =            0   itfix =              0   izfix =           0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

True or False for whether dose rates are included in output

Output includes tabulated dose rates for different times and altitudes

Number of dose rates to be reported

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =      defin2   outfil =      usrout   nstr =           4
lat =          0.000   lon =          0.000   tmzone =       0.0
iyear =         2002   imonth =           3   iday =          21
zstart =       0.000   zstop =      120.000   nz =           121
wstart =     120.000   wstop =      735.000   nwint =       -156
tstart =      12.000   tstop =       20.000   nt =             5
lzenit =           F   alsurf =       0.100   psurf =     -999.0
o3col =      300.000   so2col =       0.000   no2col =     0.000
taucld =       0.000   zbase =        4.000   ztop =       5.000
tauaer =       0.235                          alpha =      1.000
dirsun =       1.000                          difup =      1.000
zout =         0.500
lirrad =           F
lrates =           F
ljvals =           T   ijfix =            0   nmj =            7
iwfix =            0   itfix =            0   izfix =          0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Output photolysis rates for reaction ijfix at different times and altitudes

Number of photolysis rates to be reported

True or False for whether photolysis rates are included in output

TUV Fortran Program

```
TUV inputs:
==================================================================
inpfil =      defin2  outfil =      usrout  nstr =            4
lat =          0.000  lon =          0.000  tmzone =        0.0
iyear =         2002  imonth =           3  iday =           21
zstart =       0.000  zstop =      120.000  nz =            121
wstart =     120.000  wstop =      735.000  nwint =        -156
tstart =      12.000  tstop =       20.000  nt =              5
lzenit =           F  alsurf =       0.100  psurf =      -999.0
o3col =      300.000                        no2col =      0.000
taucld =       0.000
tauaer =       0.235
dirsun =       1.000
zout =         0.500
lirrad =           F
lrates =           F
ljvals =           T
iwfix =            0  itfix =            0  izfix =           0
==================================================================
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
```

Output spectral irradiance or spectral actinic flux at wavelength = iwfix for different times and altitudes

Output spectral irradiance or spectral actinic flux at time = itfix for different altitudes and wavelengths

Output spectral irradiance or spectral actinic flux at altitude = izfix for different times and wavelengths

TUV Fortran Program

Make one change to input:

Type: outfil
Type: screen

This will give output on screen instead of in an output file.

```
 Type ?variable for help on a variable, or
 <enter> = keep these settings, or
 Type variable name to change (lower case):
outfil
 write new value for outfil
screen
```

Then push “return” (or “enter”)
And “enter” again (that is, do not save input file
The program calculates and prints output.

TUV Output

```
 done: loading inputs
 calculating....
 equally spaced z-grid
step =     1 sza =     1.829 Earth-sun factor =  1.0076792
step =     2 sza =    28.200 Earth-sun factor =  1.0076326
step =     3 sza =    58.205 Earth-sun factor =  1.0075837
step =     4 sza =    88.211 Earth-sun factor =  1.0075371
step =     5 sza =   118.216 Earth-sun factor =  1.0074904
Spectral actinic flux, quanta cm-2
values at z =      0.500 km
Columns: wavelength (nm), times (hr
    wc, nm     12.000     14.000     16.000     18.000     20.000
    sza =       1.829     28.200     58.205     88.211    118.216
  120.7000  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  121.6500  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  122.1000  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  122.7000  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  123.4500  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  124.2000  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
  125.0000  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

Five time steps and solar zenith angles

Actinic Flux at z=0.5 km, different wavelengths and 5 times

TUV Output

```
Photolysis rate coefficients, s-1
   1 = O3 -> O2 + O(1D)
   2 = H2O2 -> 2 OH
   3 = NO2 -> NO + O(3P)
   4 = NO3 -> NO + O2
   5 = NO3 -> NO2 + O(3P)
   6 = CH2O -> H + HCO
   7 = CH2O -> H2 + CO
values at z =       0.500 km
Columns: time, sza, photo-reactions
time, hrs.  sza, deg.          1          2          3          4          5          6          7
   12.0000      1.829  5.292E-05  9.341E-06  1.196E-02  2.523E-02  2.009E-01  4.120E-05  5.888E-05
   14.0000     28.200  4.013E-05  8.186E-06  1.121E-02  2.463E-02  1.956E-01  3.565E-05  5.314E-05
   16.0000     58.205  1.112E-05  4.203E-06  7.629E-03  2.070E-02  1.618E-01  1.701E-05  3.040E-05
   18.0000     88.211  8.195E-08  1.039E-07  3.240E-04  9.924E-04  7.680E-03  2.834E-07  9.110E-07
   20.0000    118.216  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00  0.000E+00
```

Photolysis rates of 7 reactions at 5 time steps and solar zenith angles

Exercises

Modify input section:

1) Change latitude and longitude to location of the dust storm
   Lat = 28N   Lon = 73 E
2) Change date to time of dust storm
   2010-04-21
3) Change start and stop time to go from morning to late afternoon
   tstart=0, tstop=14
   You could also change the number of times to print out
4) Change the aerosol optical depth (tauaer) to the value for the dust storm
   tauaer = 1.5
5) Change the Angstrom component (alpha) to the value for the dust storm
   alpha = 1.0
6) Change the altitude to compare results from near the surface to near the top of the troposphere
   zout = 12 km

How much do the mid-day photolysis rates change from one step to the next?

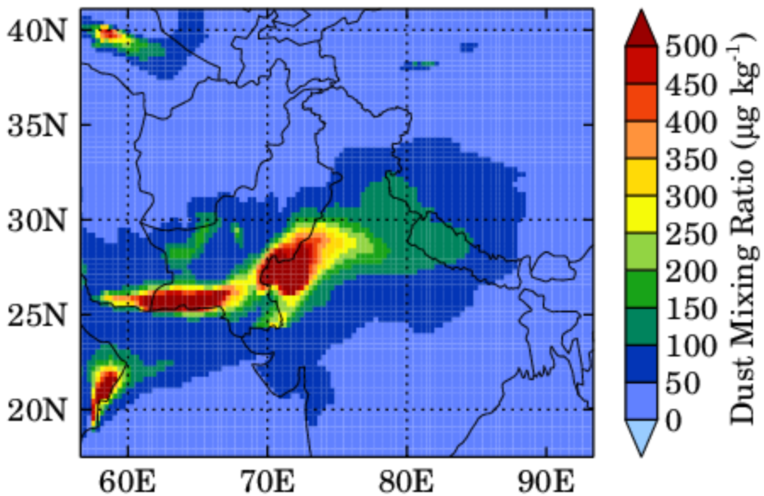
WRF-Chem Sensitivity Simulations

1. Base Case – with Dust emissions and j-values affected = Dust_J
2. No Dust emissions Case = No Dust
3. Dust emissions with J-values and Heterogeneous reactions (no relative humidity effect) = Dust_JH_NoRH
4. Dust emissions with J-values and Heterogeneous reactions (with relative humidity effect) = Dust_JH

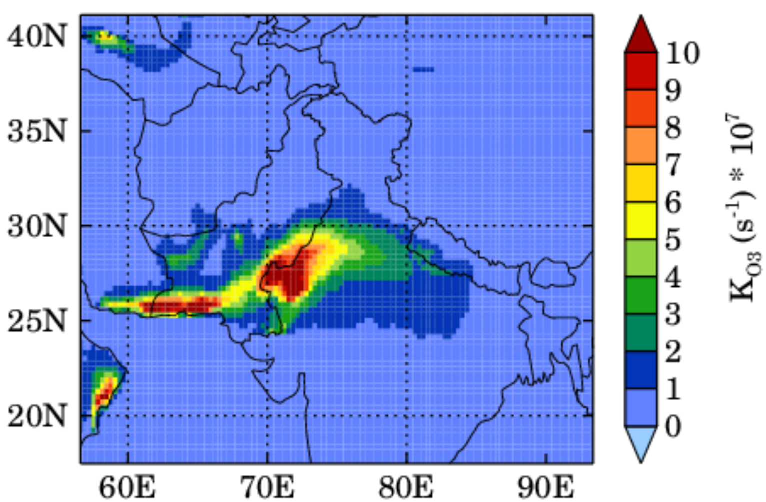
Add 12 Heterogeneous Reactions in WRF-Chem

Reaction	γ_{dry}	RH dependence
O_3 + Dust → P	2.7 x 10^{-5}	Cwiertny et al. (2008)
HNO_3 + Dust → 0.5 NO_x + P	2.0 x 10^{-3}	Liu et al. (2008)
NO_2 + Dust → P	2.1 x 10^{-6}	-
NO_3 + Dust → P	0.1	-
N_2O_5 + Dust → P	0.03	-
OH + Dust → 0.05 H_2O_2 + P	0.18	Bedjanian et al. (2013a)
HO_2 + Dust → 0.1 H_2O_2 + P	6.42 x 10^{-2}	Bedjanian et al. (2013b)
H_2O_2 + Dust → P	2 x 10^{-3}	Pradhan et al. (2010)
SO_2 + Dust → P	3.0 x 10^{-5}	Preszler Prince et al. (2007)
CH_3COOH + Dust → P	1 x 10^{-3}	-
CH_3OH + Dust → P	1 x 10^{-5}	-
CH_2O + Dust → P	1 x 10^{-5}	-

Heterogeneous Chemistry in WRF-Chem example of O_3 + dust reaction rate constant



Dust mixing ratio
17-22 April 2010



Reaction rate constant for O_3 + dust

$$k_g = \sum_{i=1}^{5} \frac{4\pi r_i D_g V N_i}{1 + K_n[\chi + \frac{4(1-\gamma)}{3\gamma}]}$$

[Heikes and Thompson, 1983]

WRF-Chem trace gases compared to observations at Nainital -- represents regional-scale concentrations

WRF-Chem reproduces observed variations in ozone and NOy at Nainital with effects of dust aerosols.