Regional-Scale Chemistry Modeling

Case Study of a Dust Storm in India

Mary Barth (NCAR), Rajesh Kumar (NCAR)

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

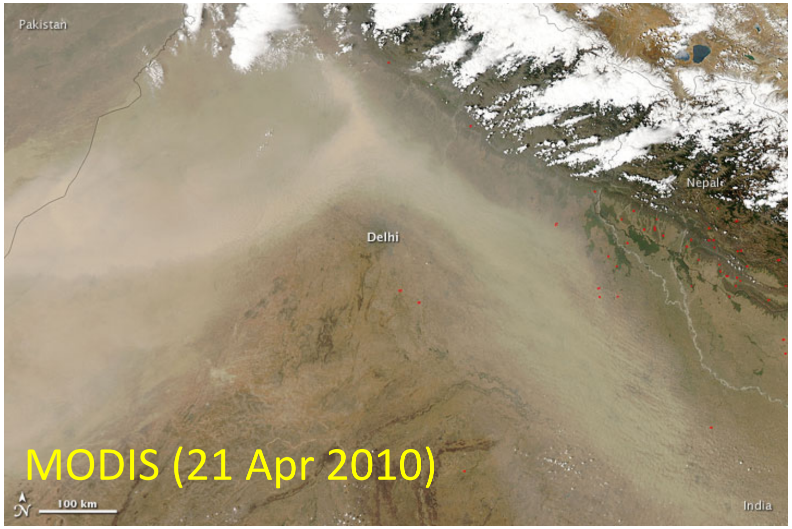
Kumar et al. (2014) *Atmos. Chem. Phys.,* Dust effects on chemistry

1. Present processes needed in chemistry transport models.
2. How to configure a model
3. How to change model – new chemical reaction, new chemical species

Exercise will be on designing model simulations

1. Forecasting for field campaign
2. Analyzing field campaign observations

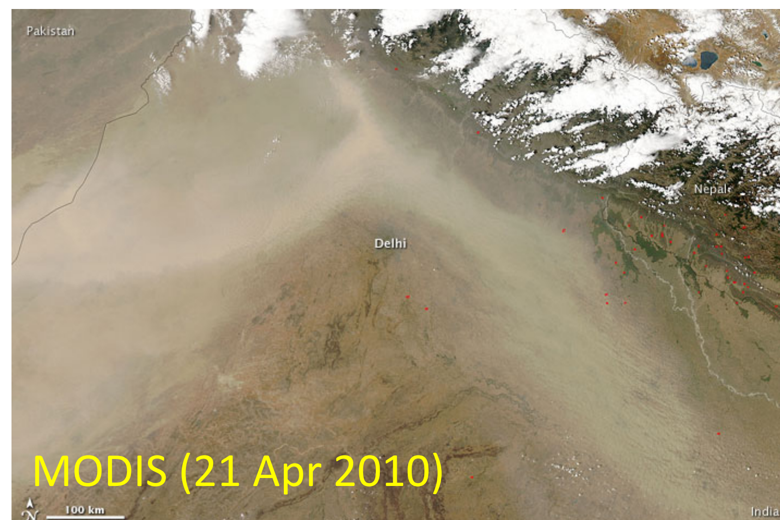
Why Model Dust Storms and Chemistry?



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

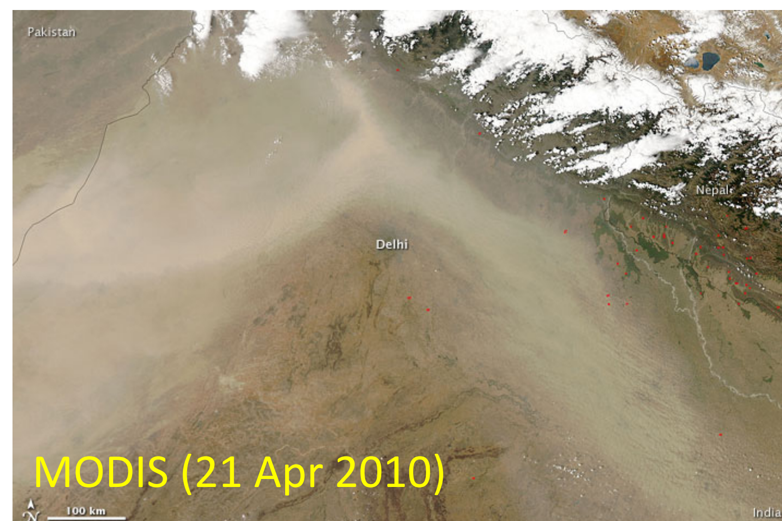
- **GOAL:** Understand the effect of these dust storms on regional scale aerosol optical properties, radiation budget and tropospheric chemistry.

What Causes the Dust to Reside over the IGP?

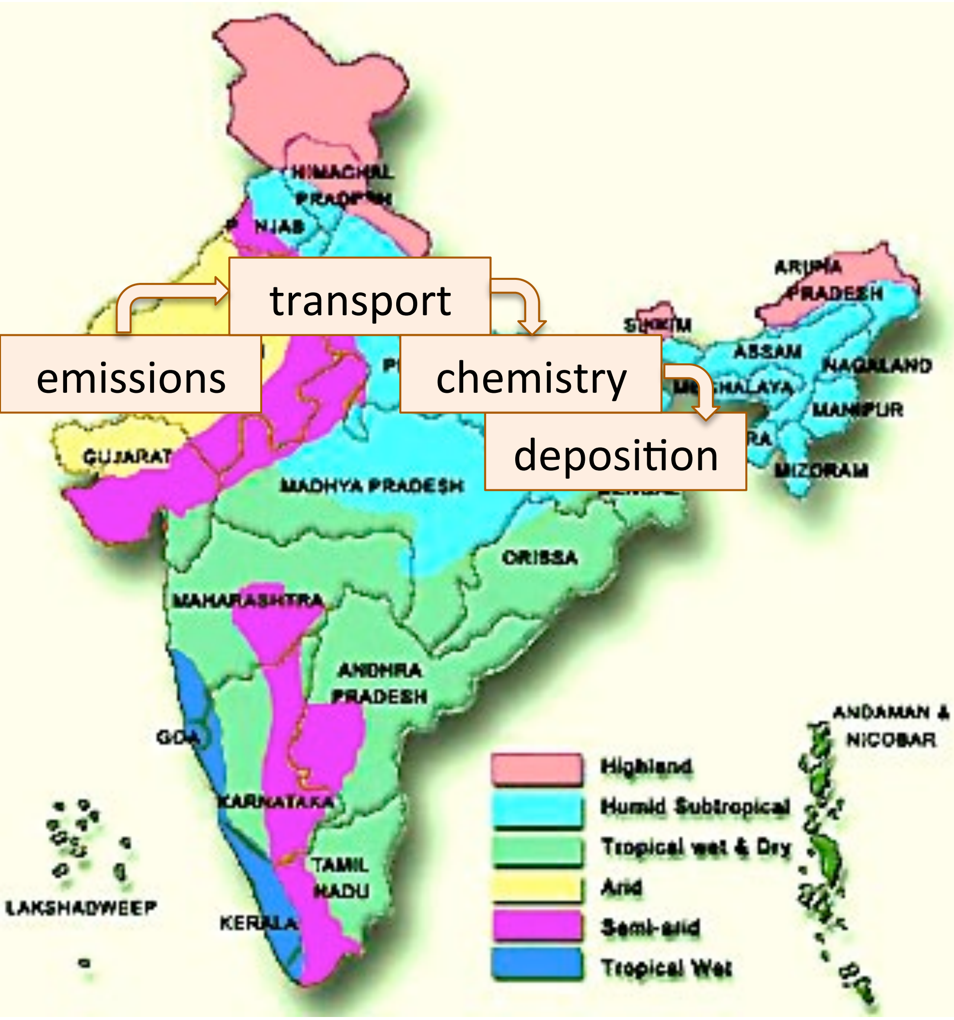


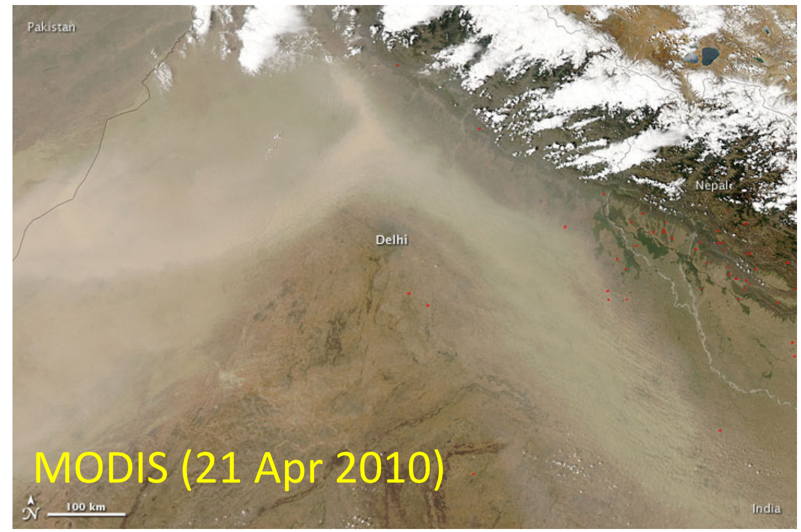
What Causes the Dust to Reside over the IGP?

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



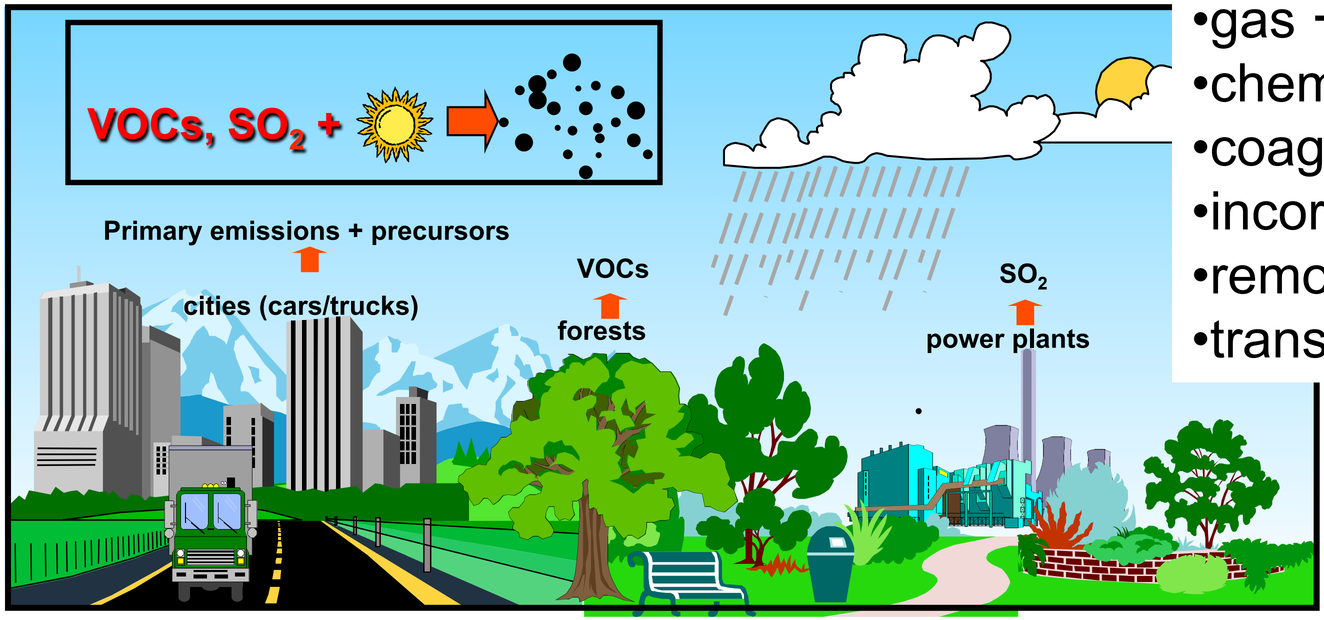
What Processes Happen from the Desert to the IGP?





Secondary (produced in atmosphere) sources of particles:

- vehicles (organics, nitrates)
- industry (sulfate, organics, nitrates, ammonium)
- plants (organics)
- agriculture (ammonium, nitrate)



Atmospheric processes:

- gas → particle conversion
- chemical reactions
- coagulation
- incorporation into clouds
- removal by precipitation
- transport

Primary (directly emitted) sources of particles:

- vehicles (soot, organics)
- industry (soot, sulfate, organics, metals)
- construction & agriculture (soot, soil)
- sea-spray (salt)
- fires (soot and organics)

From: http://www.esrl.noaa.gov/research/themes/aerosols/pdf/AerosolProcesses.pdf

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/*
- Biomass Burning Emissions

  GFED www.globalfiredata.org/

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

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

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

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

  BEIS
  https://www.epa.gov/air-emissions-modeling/biogenic-emission-inventory-system-beis

Modeling emissions of aerosols and trace gases

- Anthropogenic Emissions
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See lecture by Sachin Ghude

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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

See lecture by Federico Fierle

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

- Gas to particle nucleation
- Aerosol growth by condensation and coagulation

<u>New Particles</u>

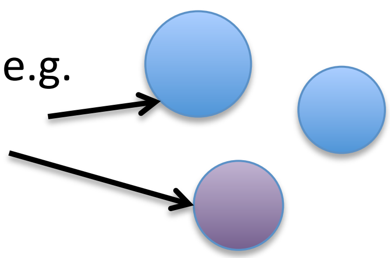
Gases, e.g. H_2SO_4, cluster together

Reach a critical size and nucleate into a particle

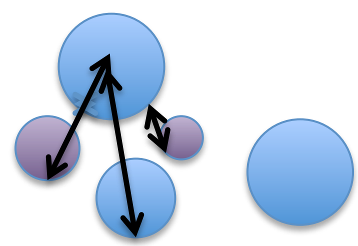
<u>Add Mass to Particles</u>

Condensation

Gases, e.g. H_2SO_4



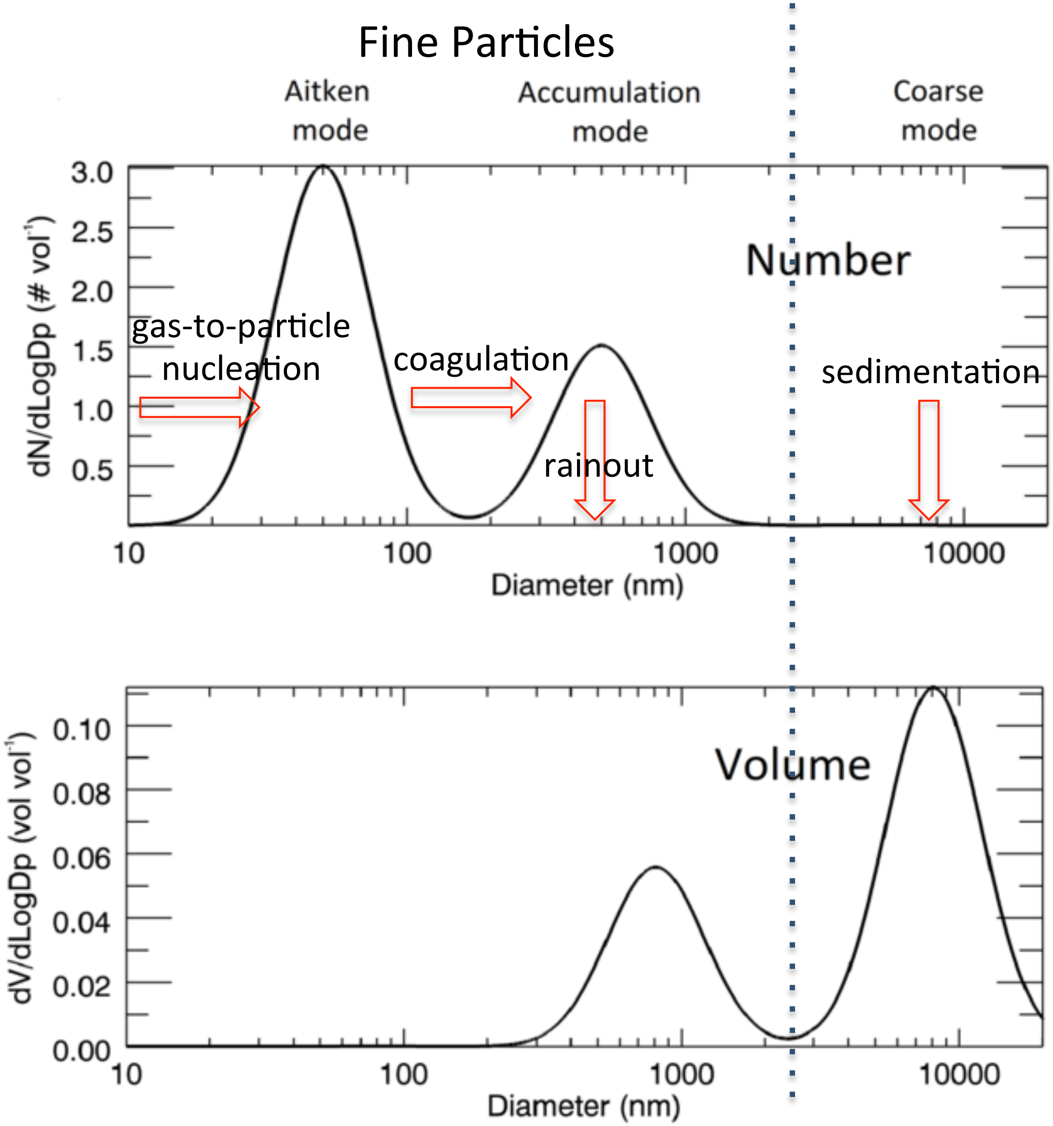
Coagulation



Aerosol Size Distribution

<u>Chemical Processes</u>

- Sulfate
- Nitrate
- Ammonium
- Organics
- Black carbon



<u>Mechanical Processes</u>

- Dust
- Sea salt
- Pollen
- Spores
- Ash (volcanos)

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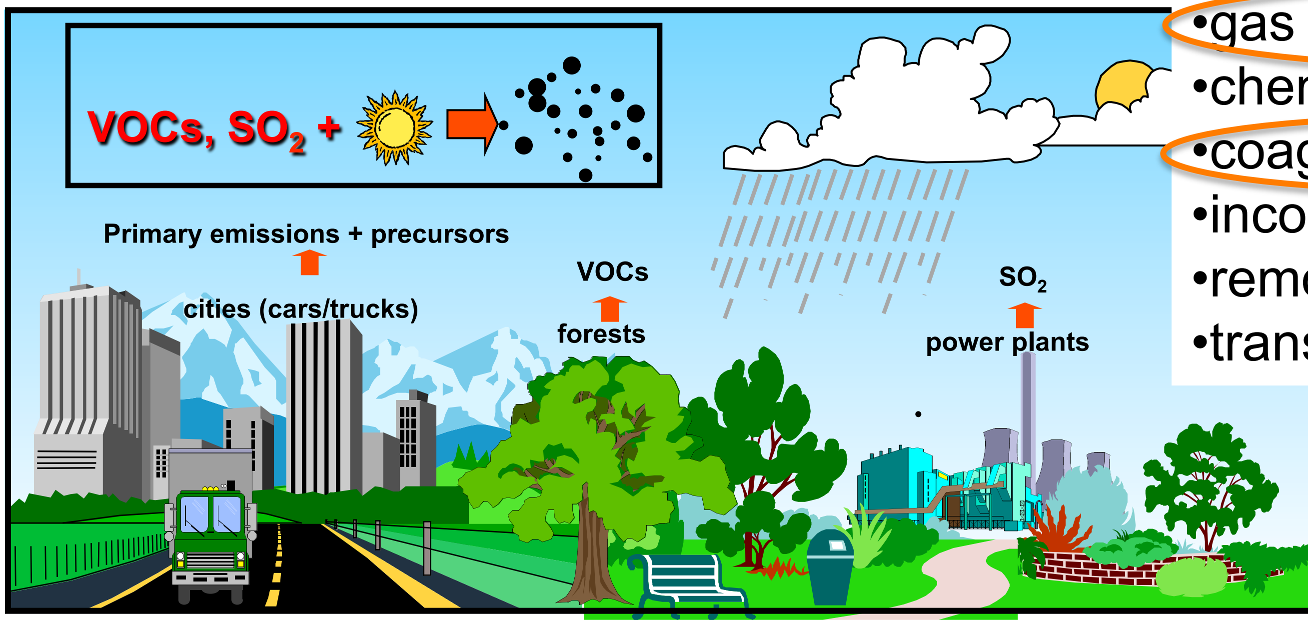

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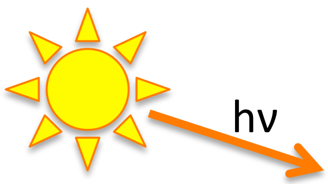
From: http://www.esrl.noaa.gov/research/themes/aerosols/pdf/AerosolProcesses.pdf

Modeling chemistry of aerosols and trace gases

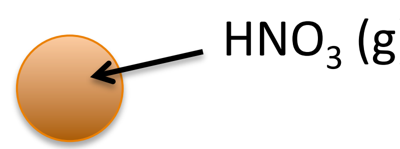
- Photodissociation reactions



$NO_2 \rightarrow NO + O$

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

Some Gas-Phase Chemical Mechanisms

- SAPRC07 or SAPRC99
- RADM or RACM
- Carbon Bond (CBM5, CBMZ)
- MOZART
- U Manchester
- Reduce Hydrocarbon
- GEOS-Chem and many others

70-200 trace gases
100s of chemical reactions

What's the difference among these mechansims?

30 trace gases
68 chemical reactions

Some Gas-Phase Chemical Mechanisms

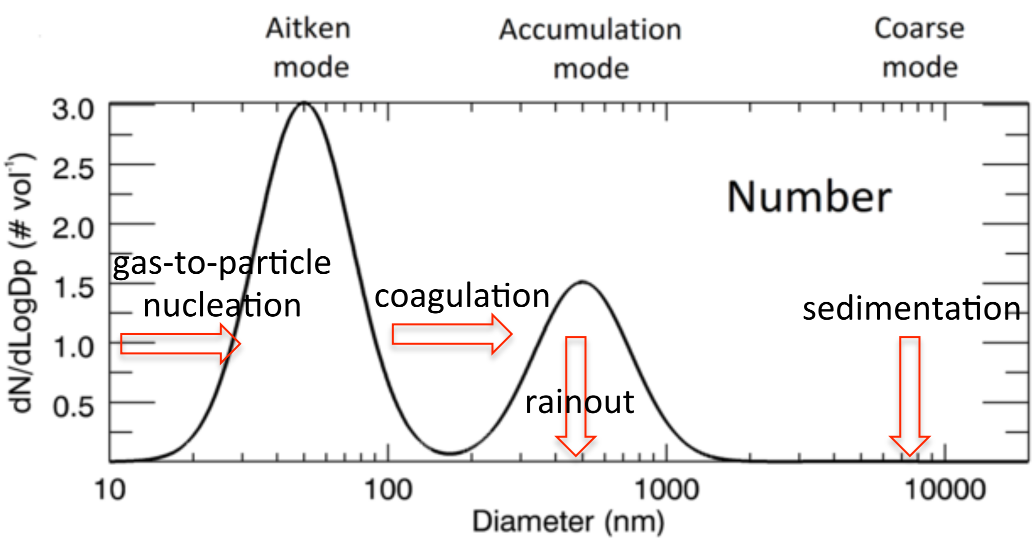
What to do if you want a new reaction added?
-- It may be easy! Especially if the kinetic pre-processor is used. KPP writes the chemistry code for you.
→ become familiar with KPP, use its box model to practice adding your new gas-phase reaction

What to do if you want another trace gas added?
-- more work! Do everything for adding a new reaction.
-- new trace gas needs to be included in dry deposition, wet deposition, and photolysis rate calculation (if it photodissociates)

- SAPRC07 or SAPRC99, RADM or RACM, Carbon Bond (CBM5, CBMZ), MOZART, U Manchester,
- Reduce Hydrocarbon
- GEOS-Chem and many others

Some Aerosol Representations

- Bulk mass mixing ratios
- Modal aerosol models
- Sectional bin models



Some Aerosol Representations

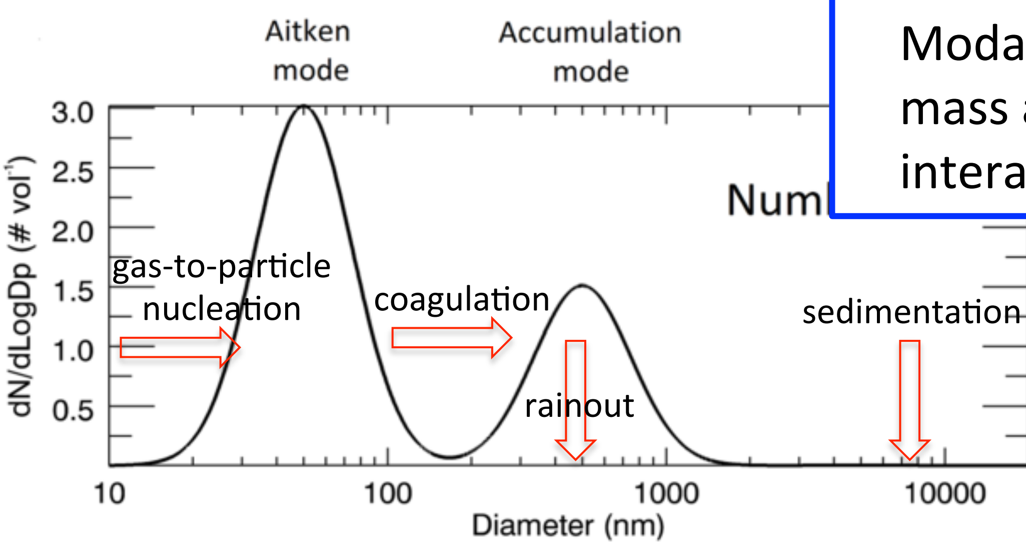
- Bulk mass mixing ratios
- Modal aerosol models
- Sectional bin models

In general:

Bulk models do not represent aerosol chemistry well (working on it, so it depends on current status of model)

Bulk models: sulfate, black carbon, organic carbon, dust (4-6 sizes), sea salt (4-6 sizes)

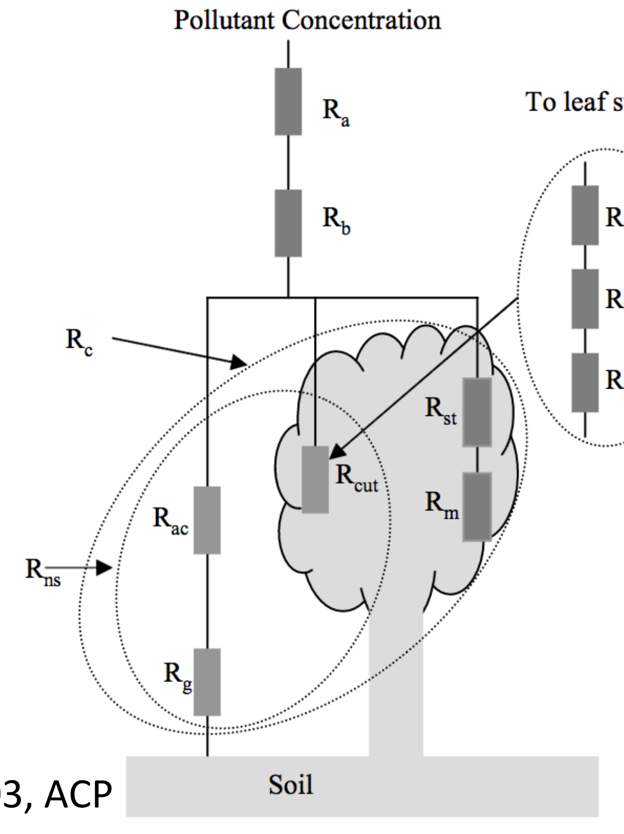
Modal and Sectional models predict mass and number → aerosol-cloud interactions are possible to study



Modeling deposition of aerosols and trace gases

- Dry Deposition
  - Deposition velocity, vegetation (canopy or not), Henry's Law constant
  - Wesely (1989) parameterization often used

$$V_d = \frac{1}{R_a + R_b + R_c}$$



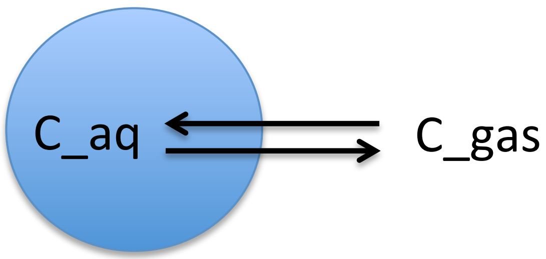
Zhang et al., 2003, ACP

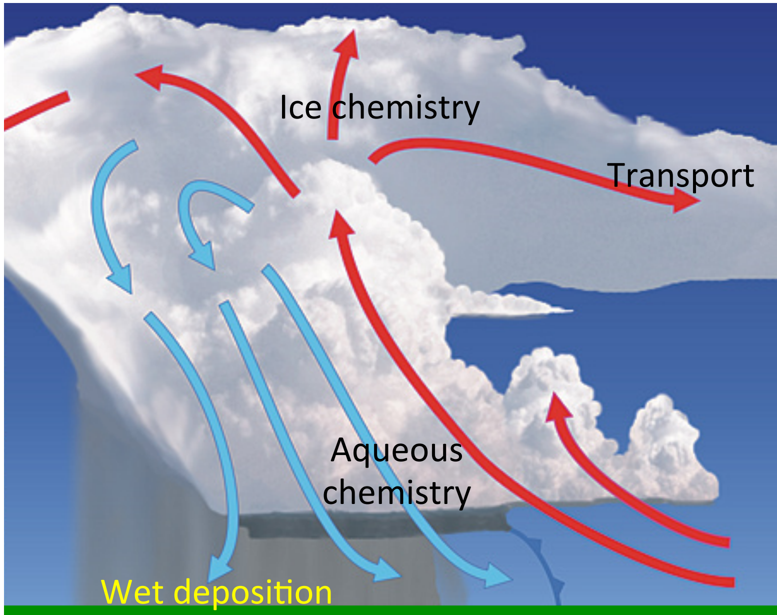
Modeling deposition of aerosols and trace gases

- Wet Deposition
  - Amount of cloud water, Henry's Law constant, production of precipitation, evaporation
- Henry's Law [mol/((liter water) atm)]

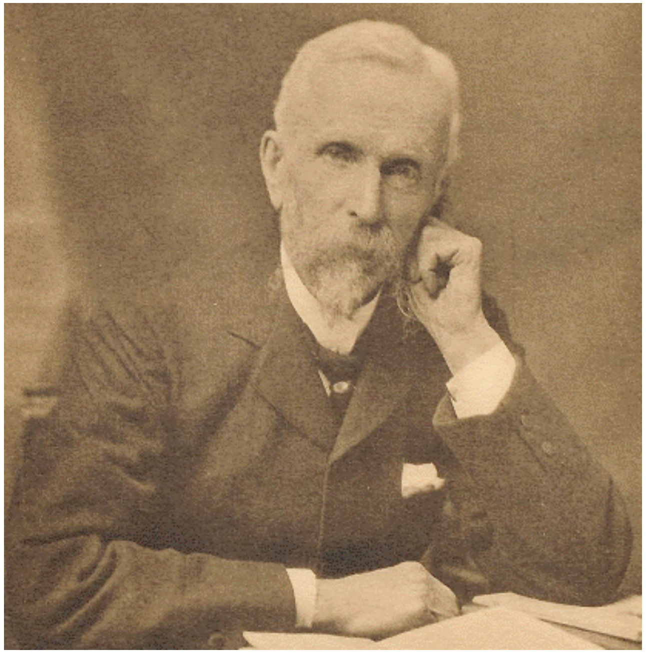
  $[C\ (aq)] = K_H\ p\_C\ (g)$ where C = trace gas

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





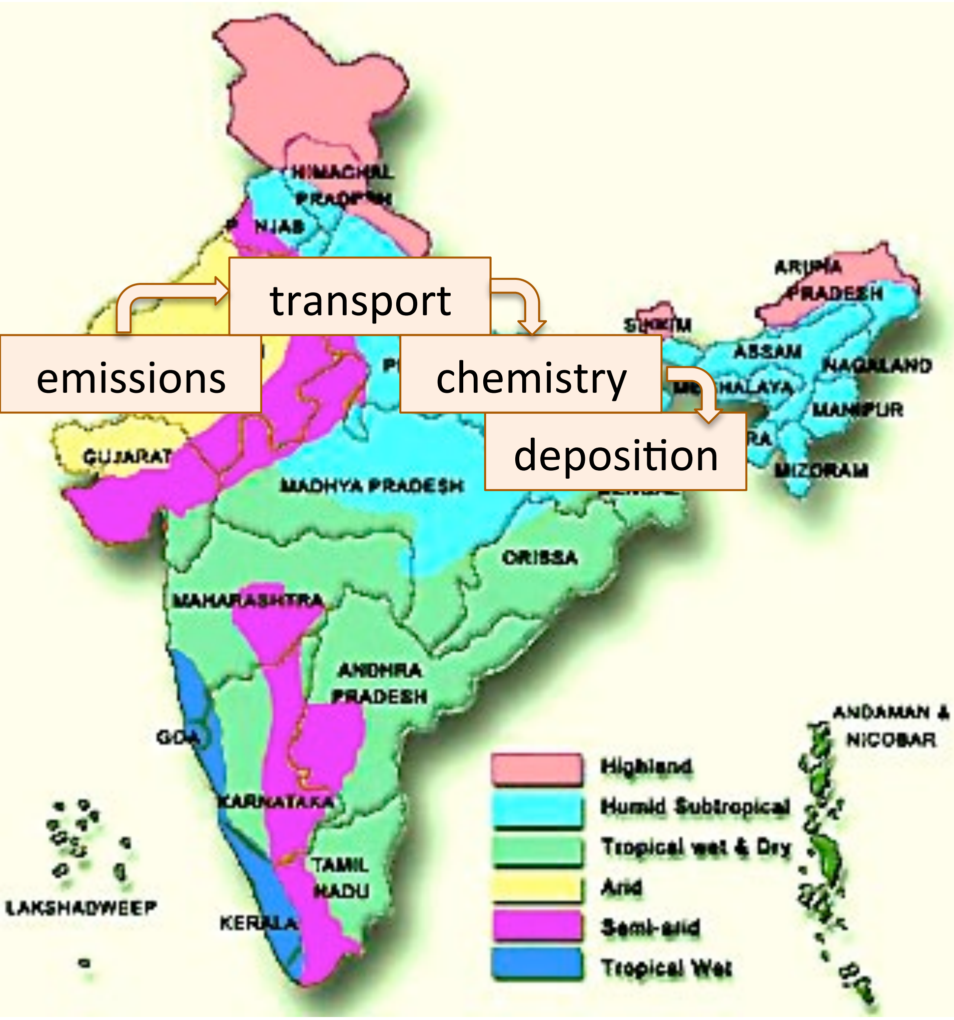
“We have in this fine dust a most beautiful illustration of how the little things in the world work great effects by virtue of their numbers.”

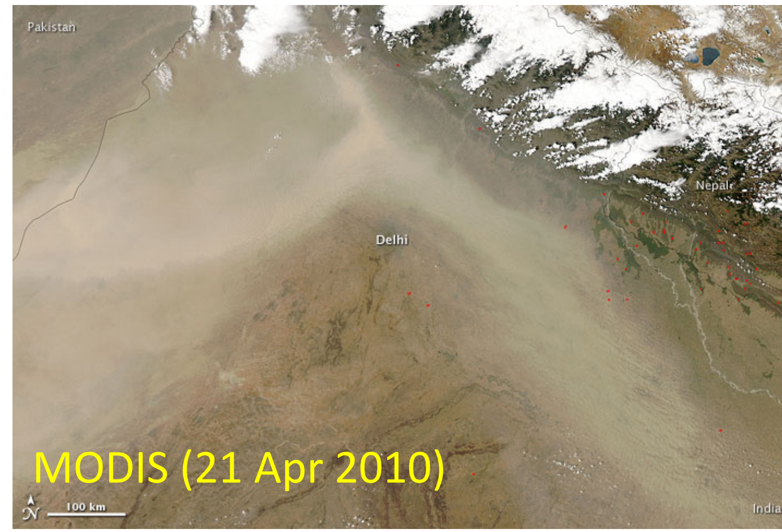


-John Aitken, 1880

http://www.iara.org/AerosolPioneers.htm

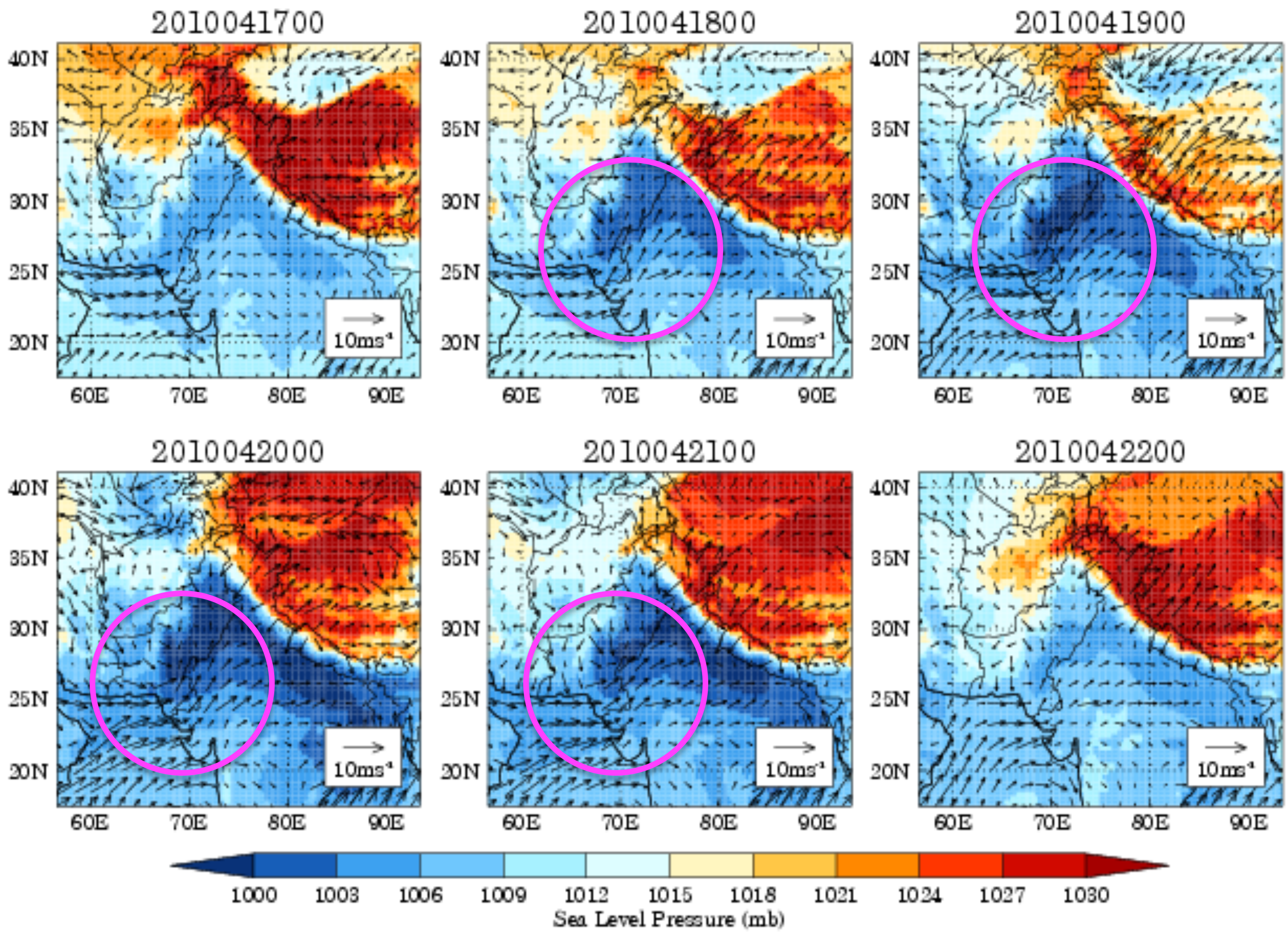
Modeling dust storm effects on aerosols and trace gases



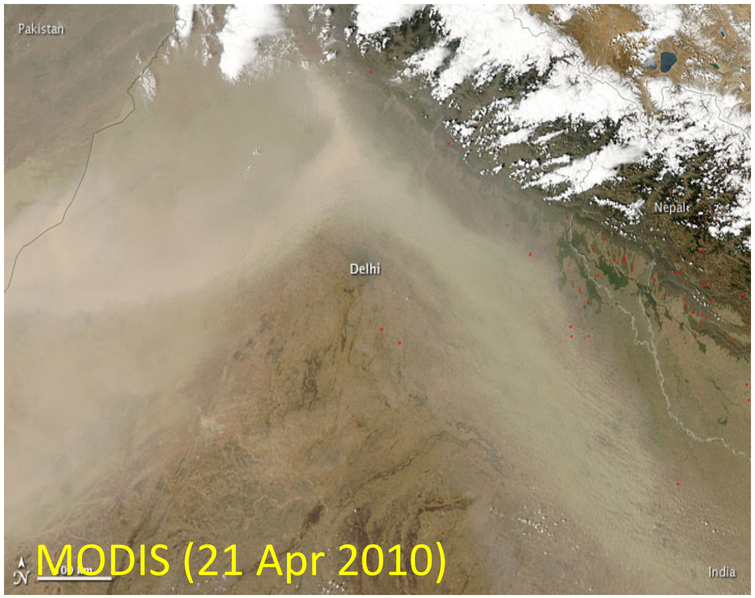


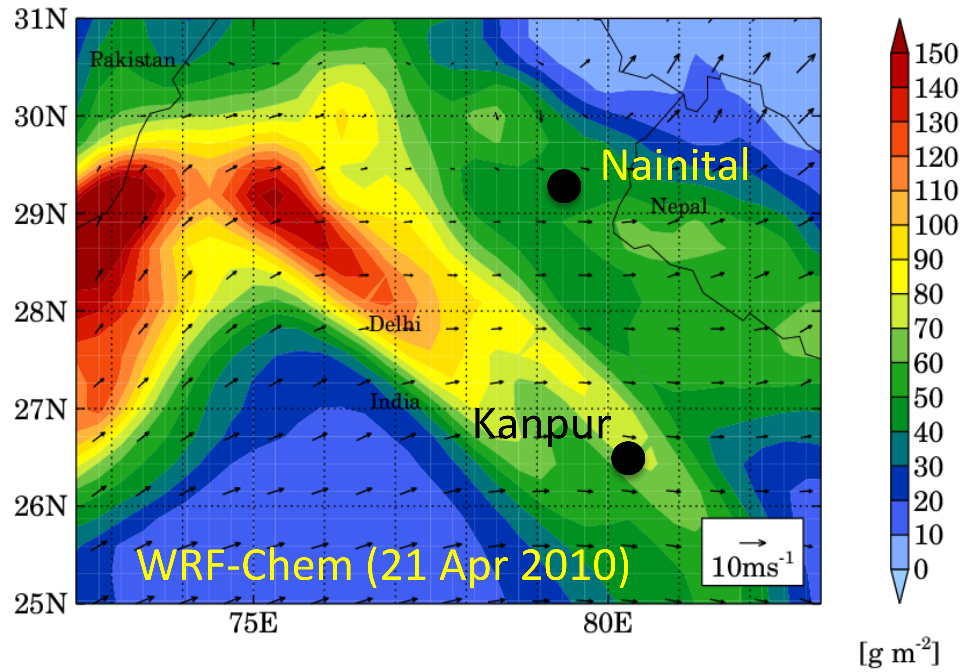
Use the Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) to learn what processes affect aerosols and trace gases

Low pressure region over the Thar Desert generated dust storm



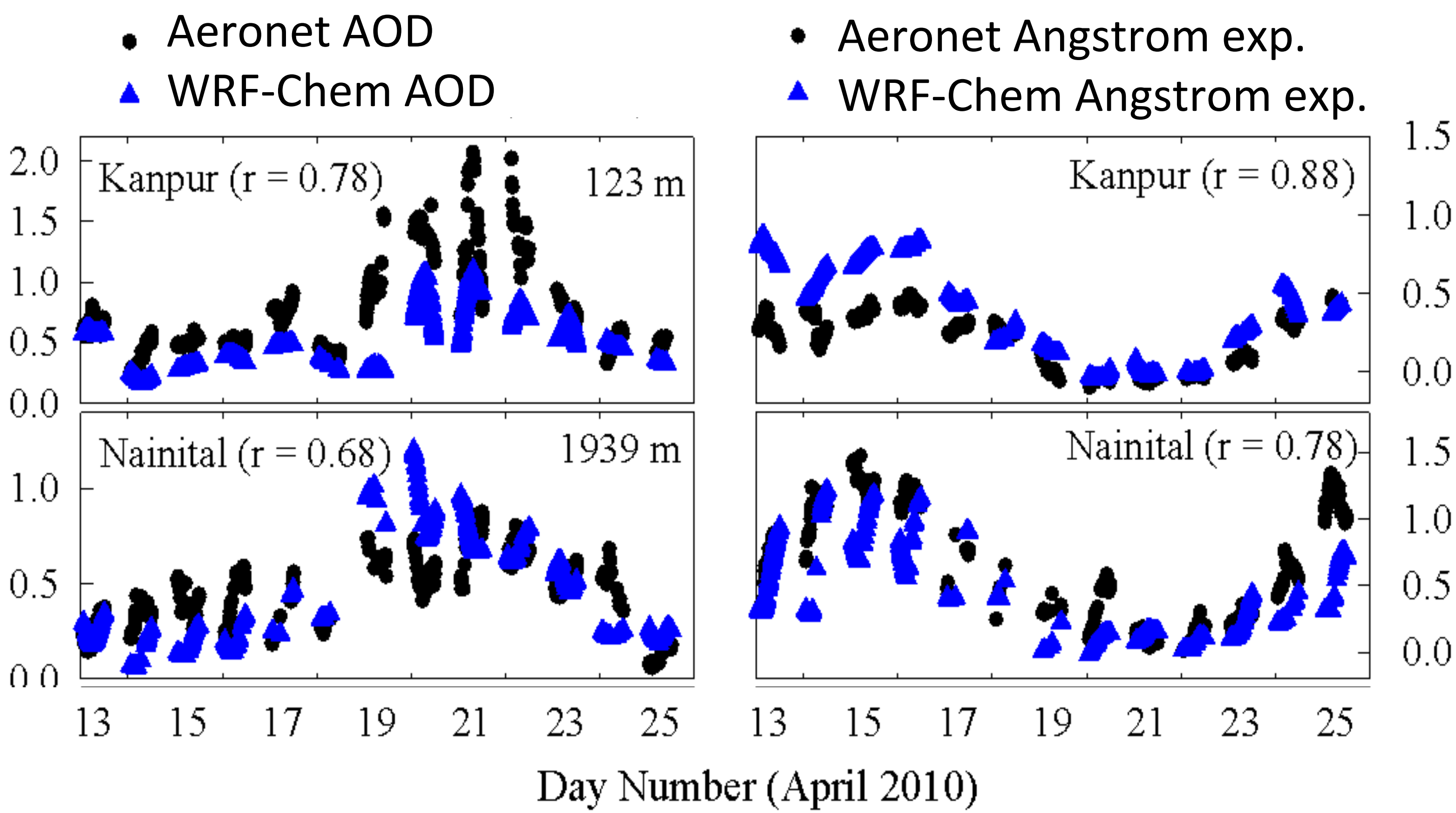
WRF-Chem captures spatial distribution of the dust storm





[Kumar et al., ACPD, 2013]

WRF-Chem captures AOD and Angstrom exponent

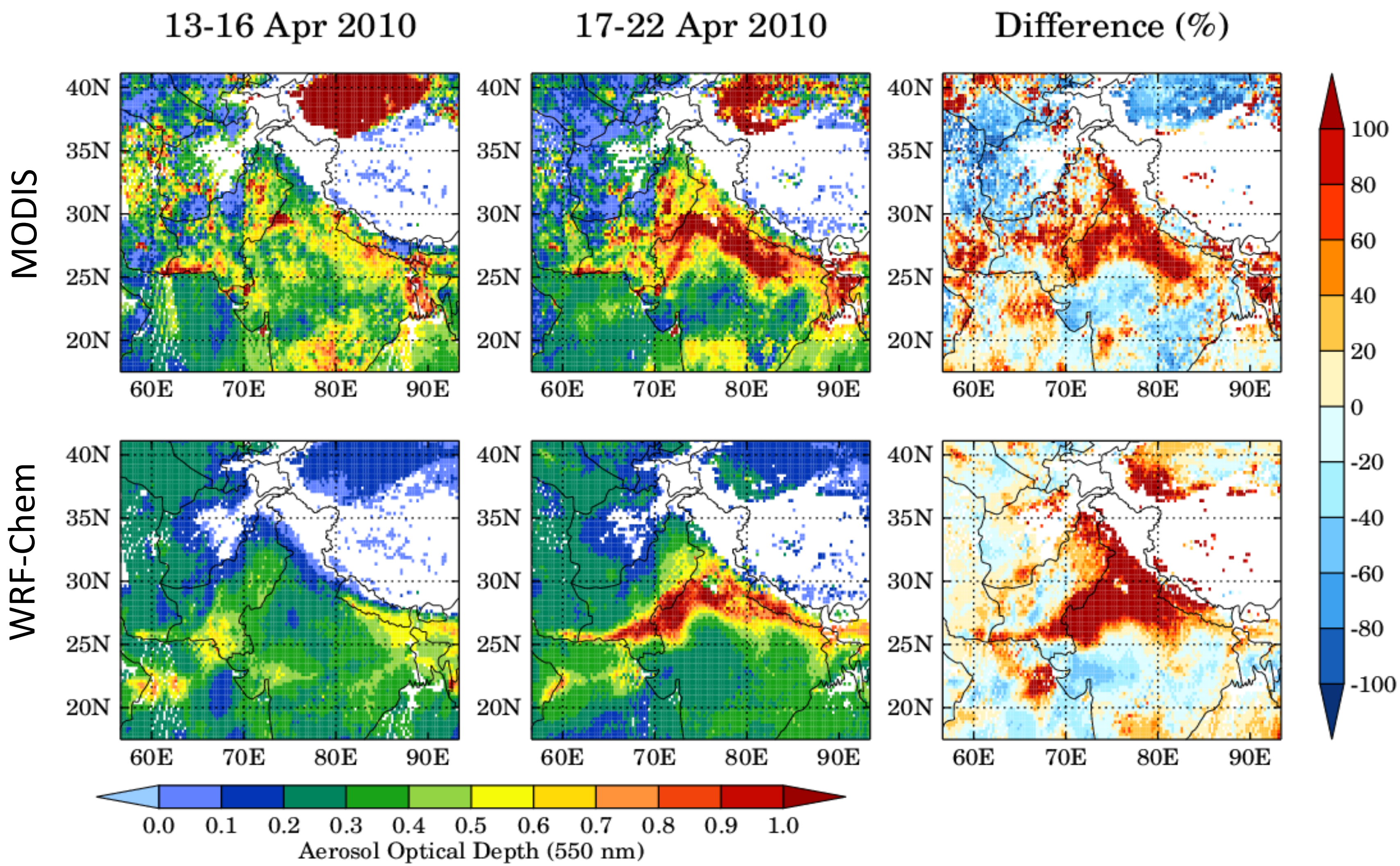


AOD – integrated extinction coefficient over a vertical column of unit cross section.

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

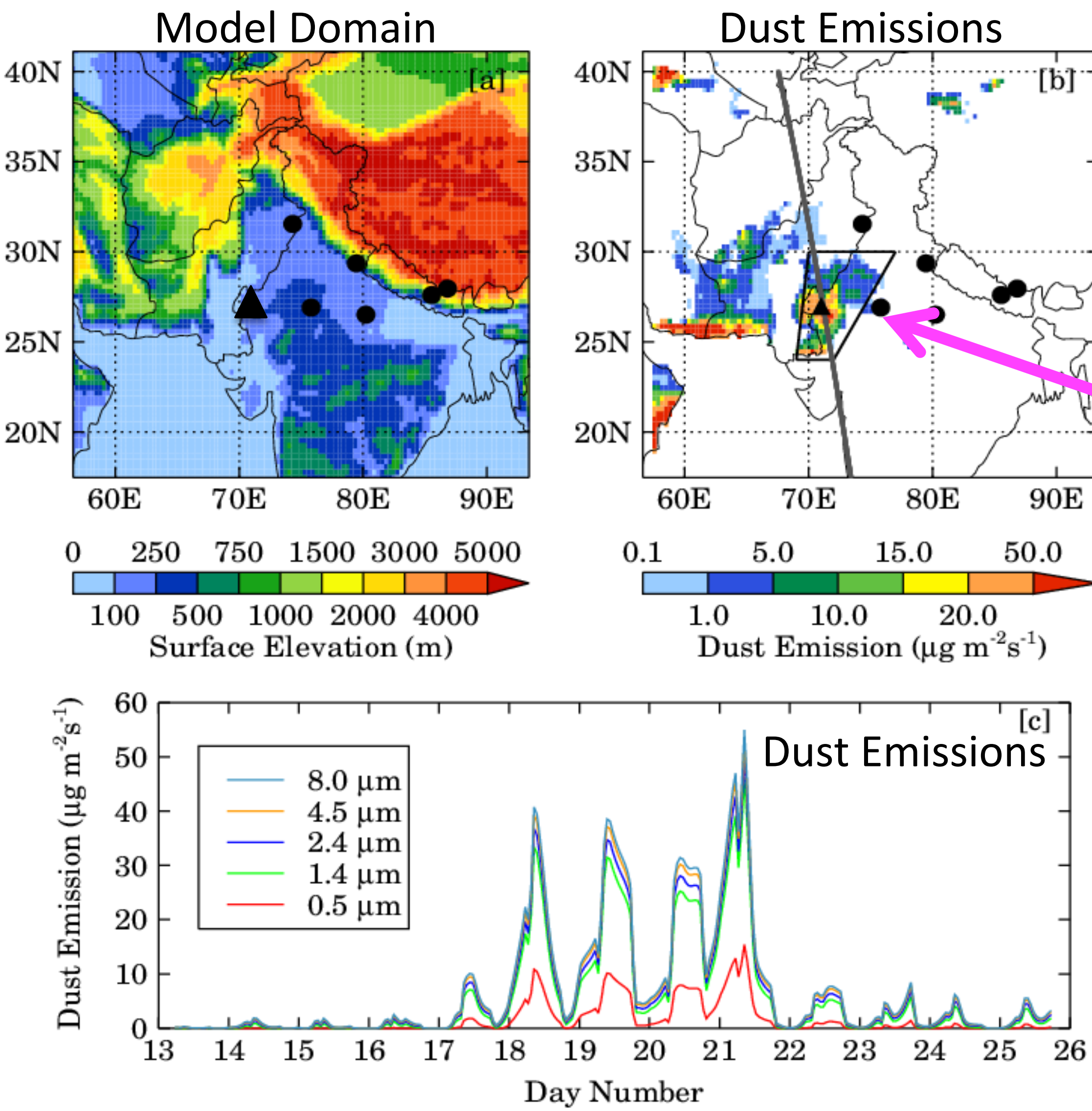
[Kumar et al., ACP, 2013]

Dust Storm almost doubled the regional aerosol loading



Trajectories for monitoring variables in an air parcel

Something new in WRF!



Start trajectories in Thar Desert

Trajectories for monitoring variables in an air parcel

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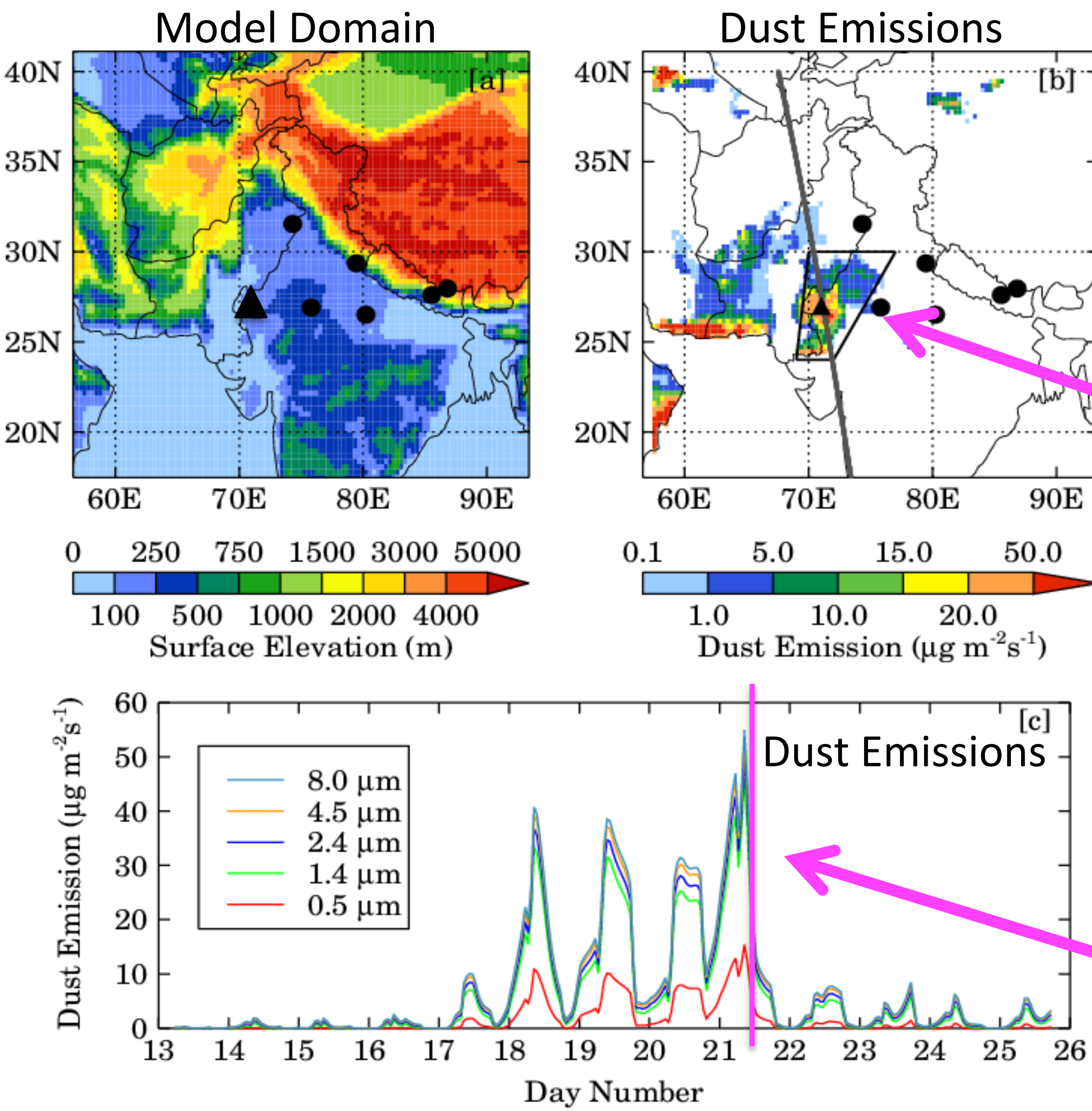


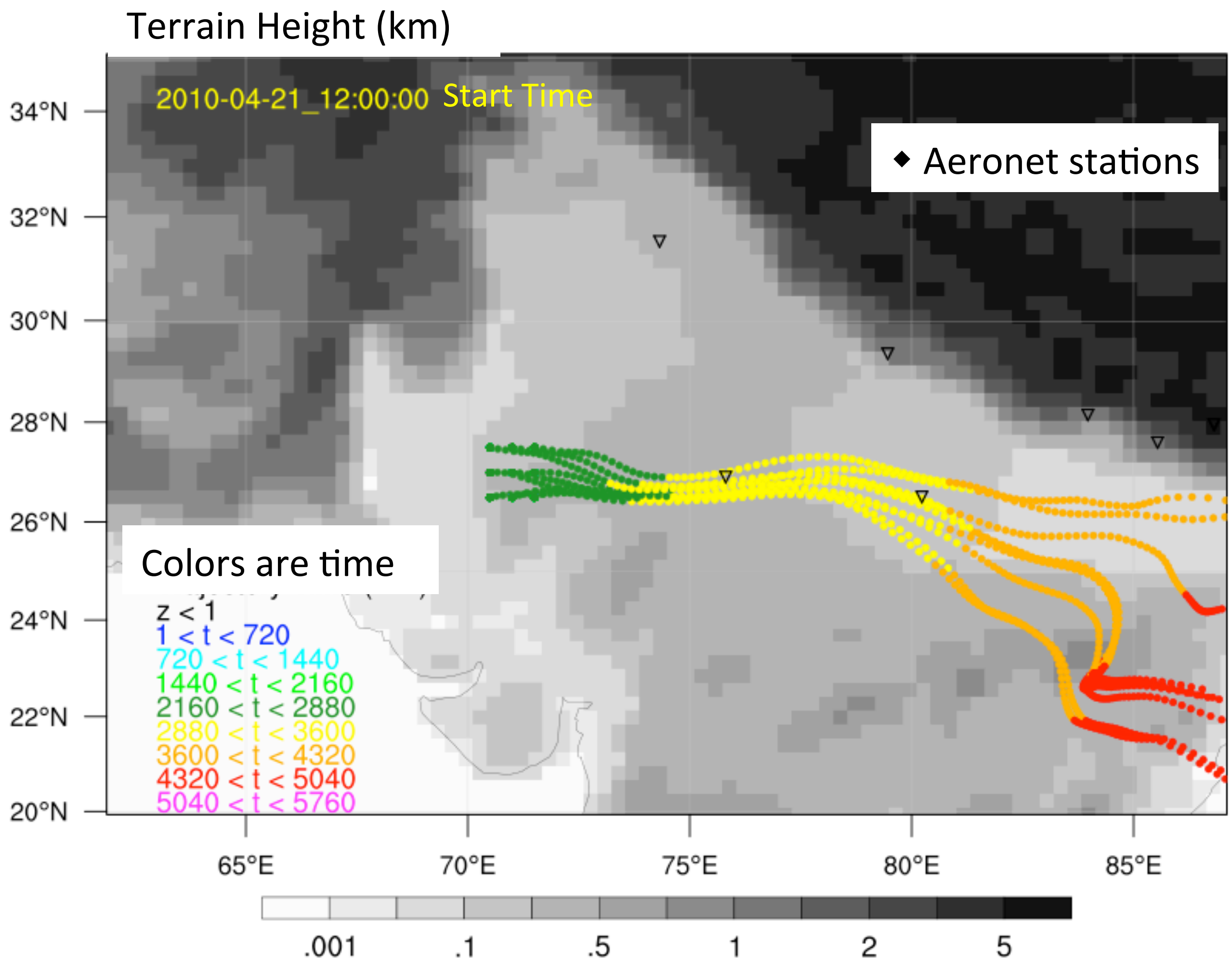
Start trajectories in Thar Desert

Started trajectories every 3 hours from 00 UTC 18 April to 21 UTC 21 April

Show results for trajectories started at 12 UTC 21 April

Trajectories for monitoring variables in an air parcel

Something new in WRF!



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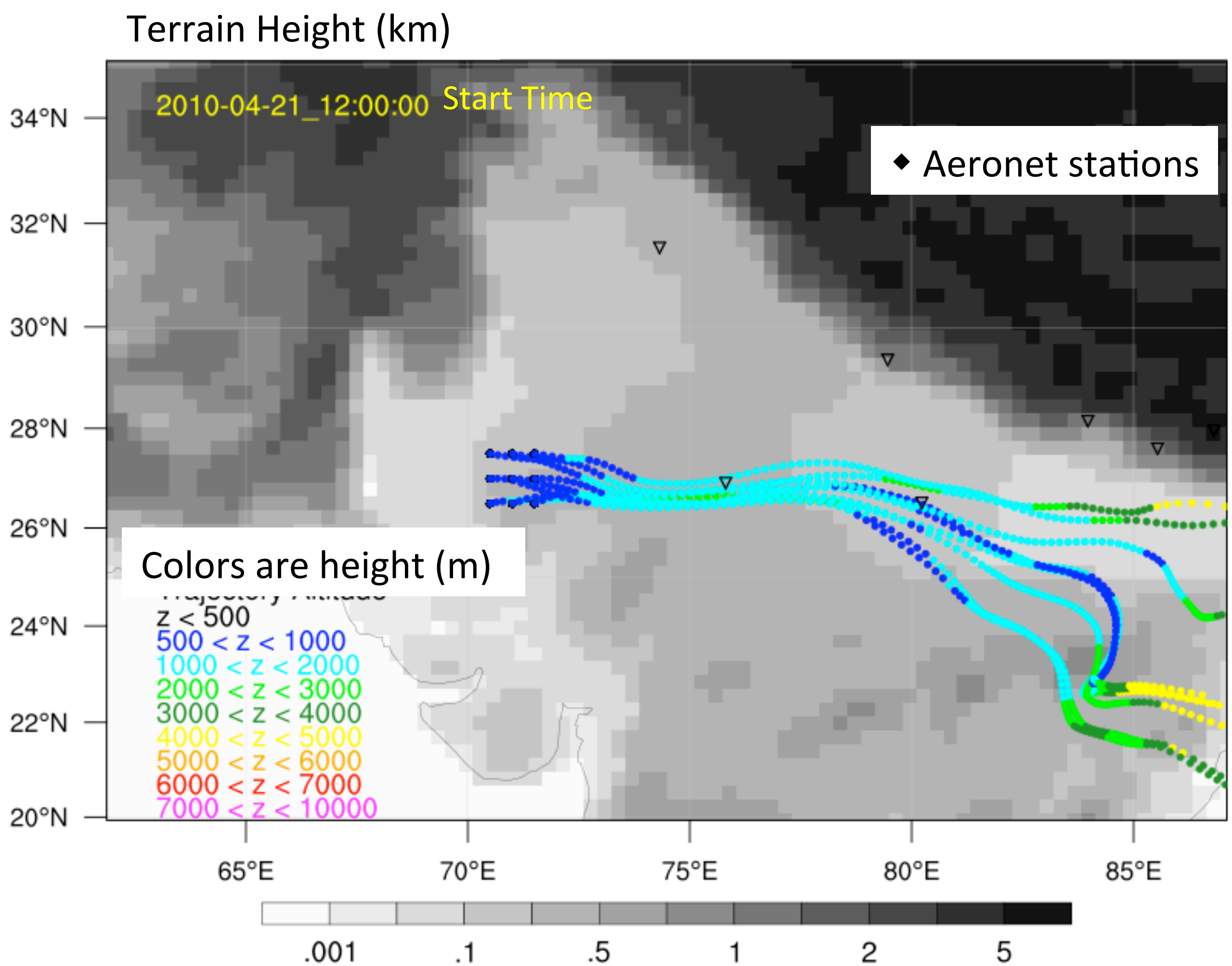

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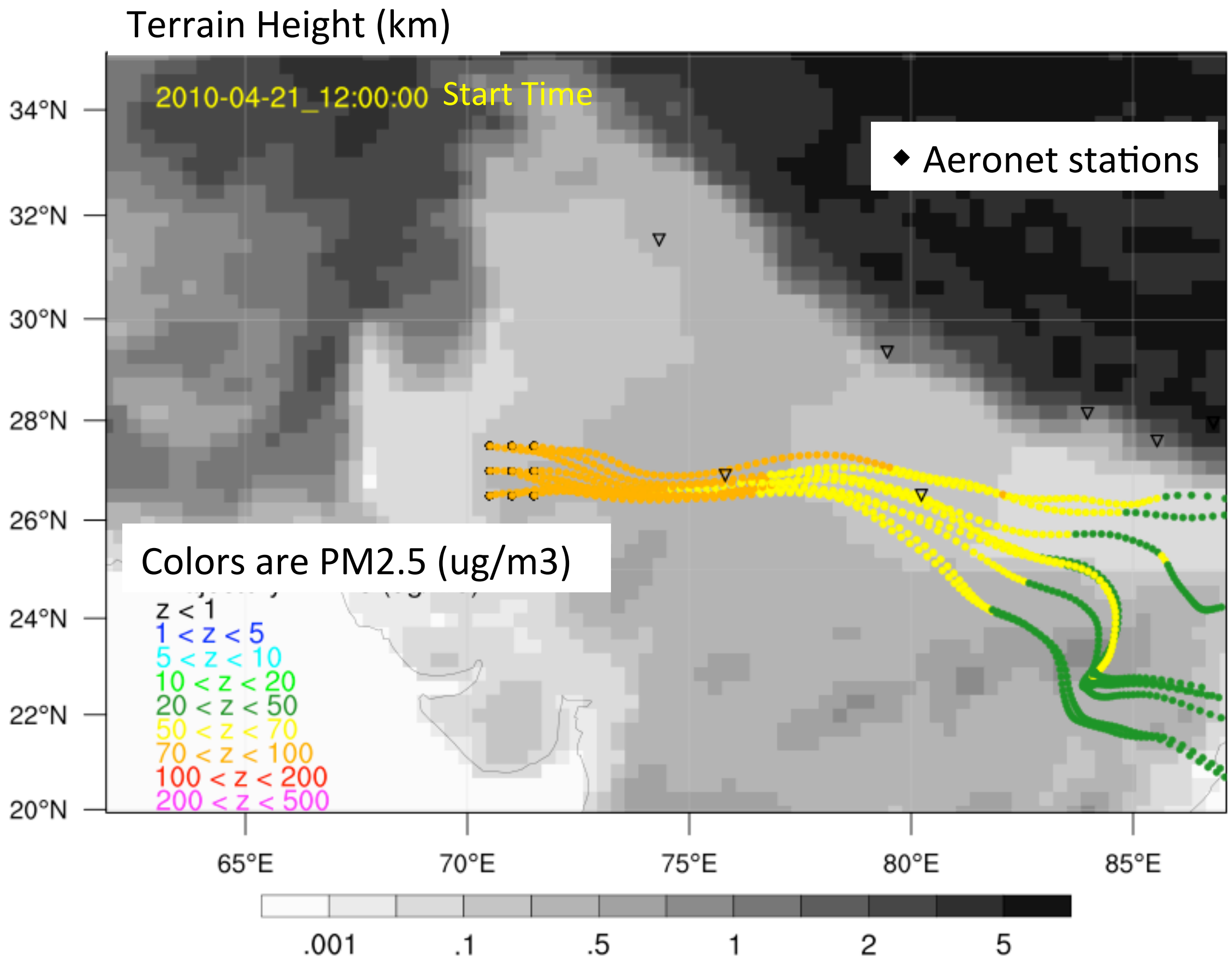
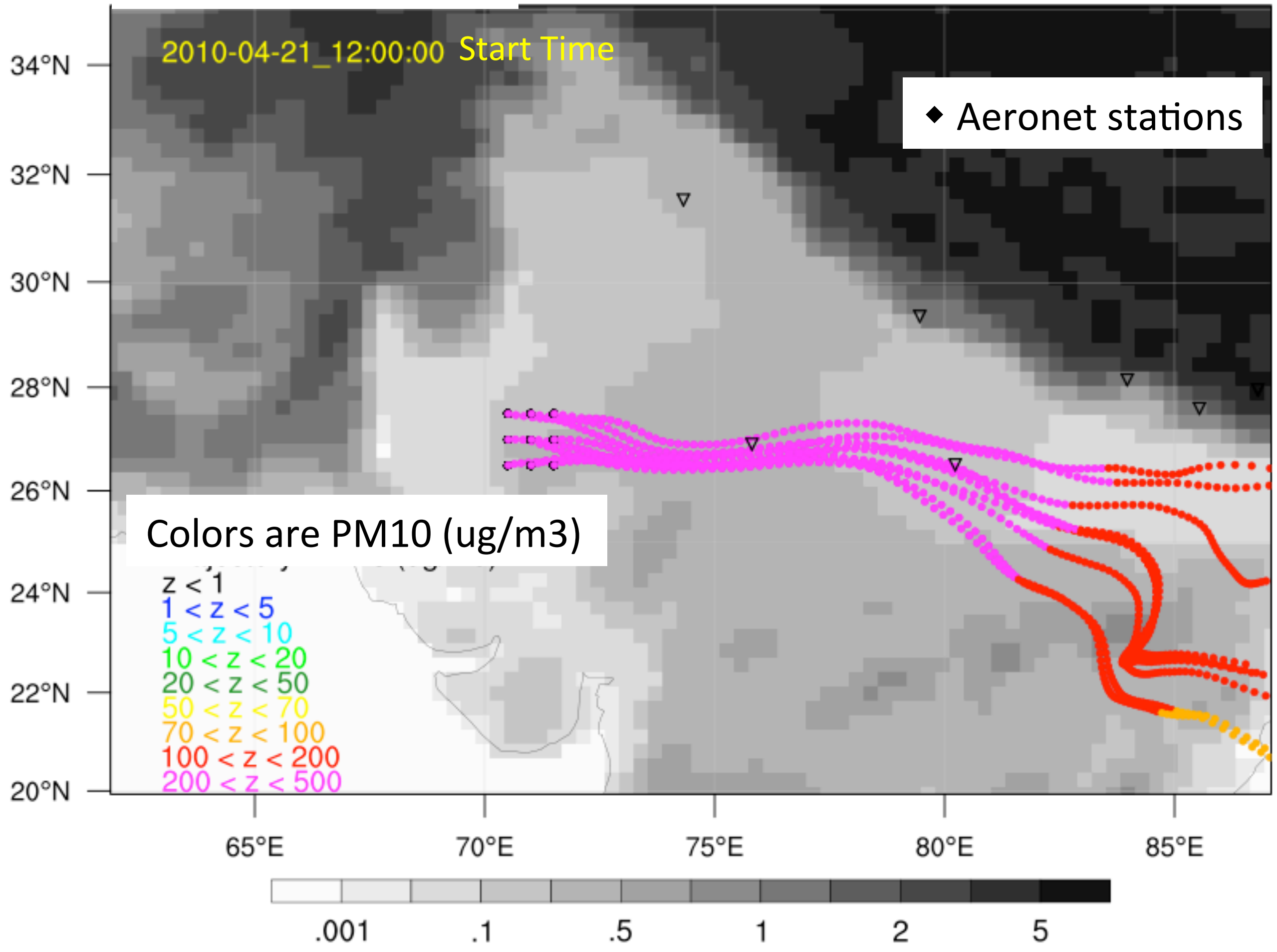


Trajectories for monitoring variables in an air parcel

Something new in WRF!

Terrain Height (km)



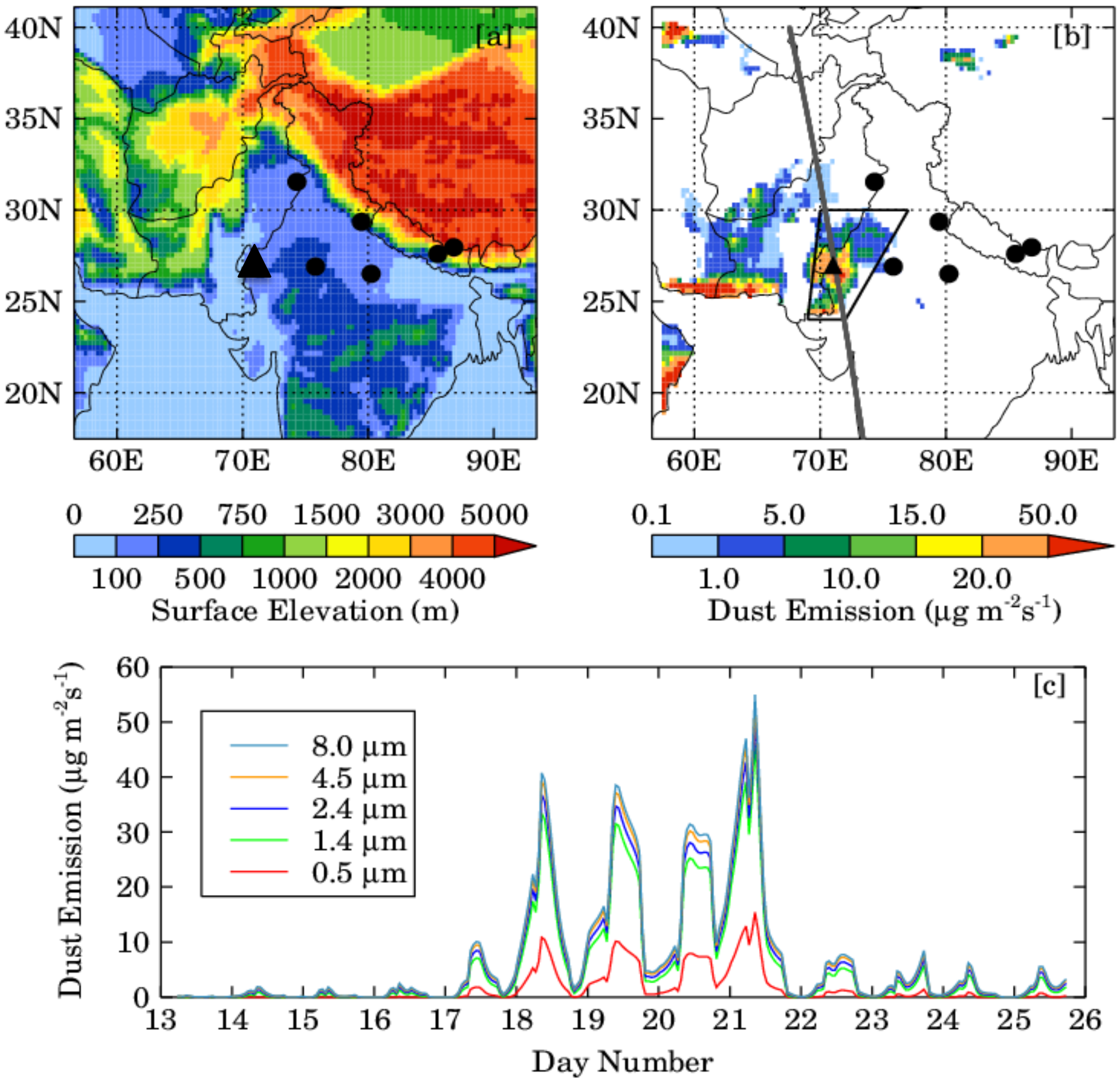
Methods for Setting Up a Regional Scale Model

Some regional scale chemistry transport models

WRF-Chem, WRF-CMAQ, CHIMERE, COSMO-ART, COSMO/MUSCAT, LOTUS-EURO, METUM UKCA, GEM-MACH

The following slides are based on WRF-Chem but should be applicable to any regional model

WRF-Chem set-up



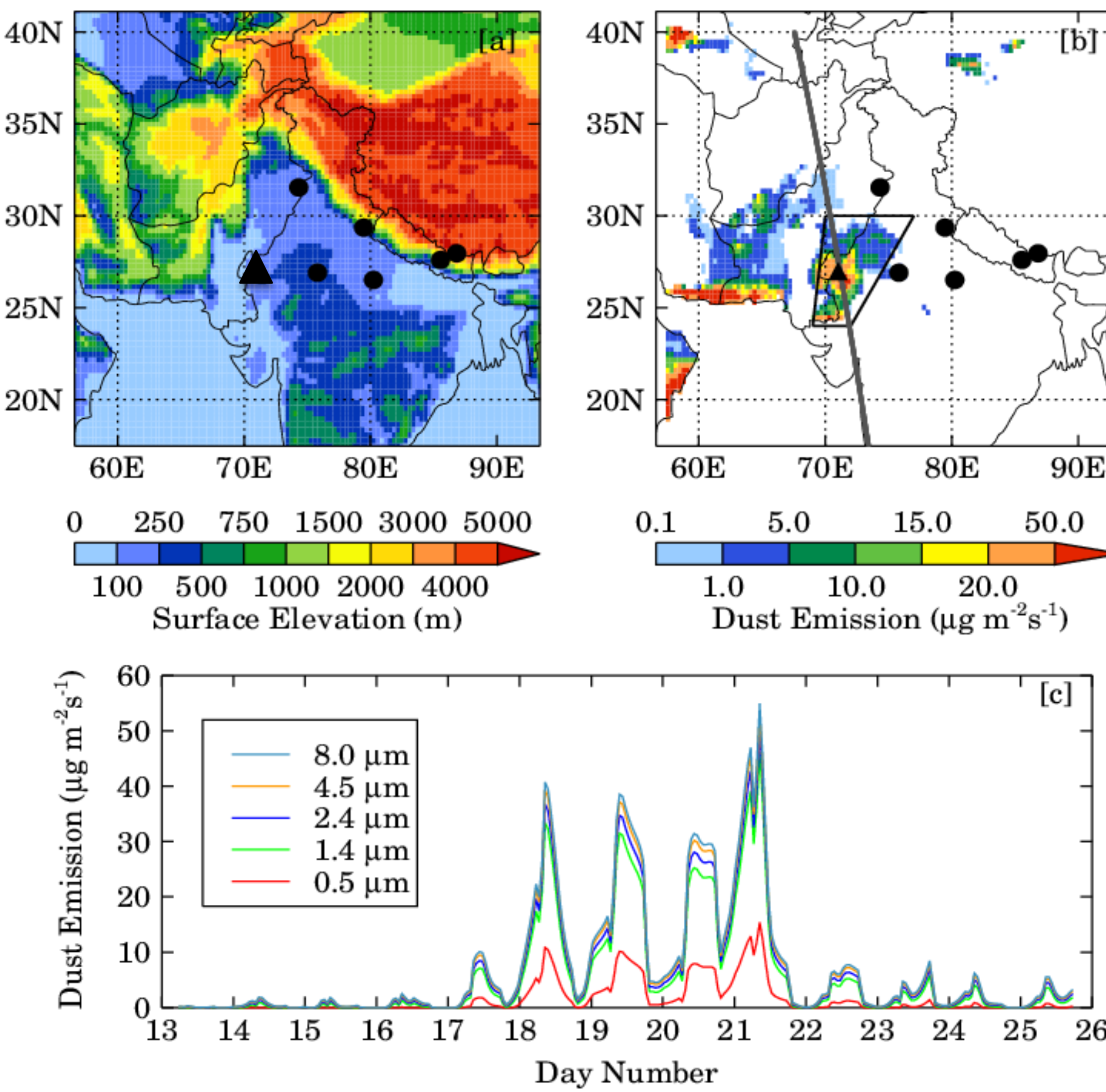
Grid spacing: 30 km
Grid points (x,y,z) = (120,90,51)
Simulation: 10-25 Apr 2010

Top of model: 10 hPa

Why so high?
With tall mountains, stratosphere is closer to ground. Need to give space for interactions between stratosphere and troposphere.

Model tops can reflect waves back region of interest. Can reduce impact with higher model top and region to absorb waves.

WRF-Chem set-up



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

Top of model: 10 hPa

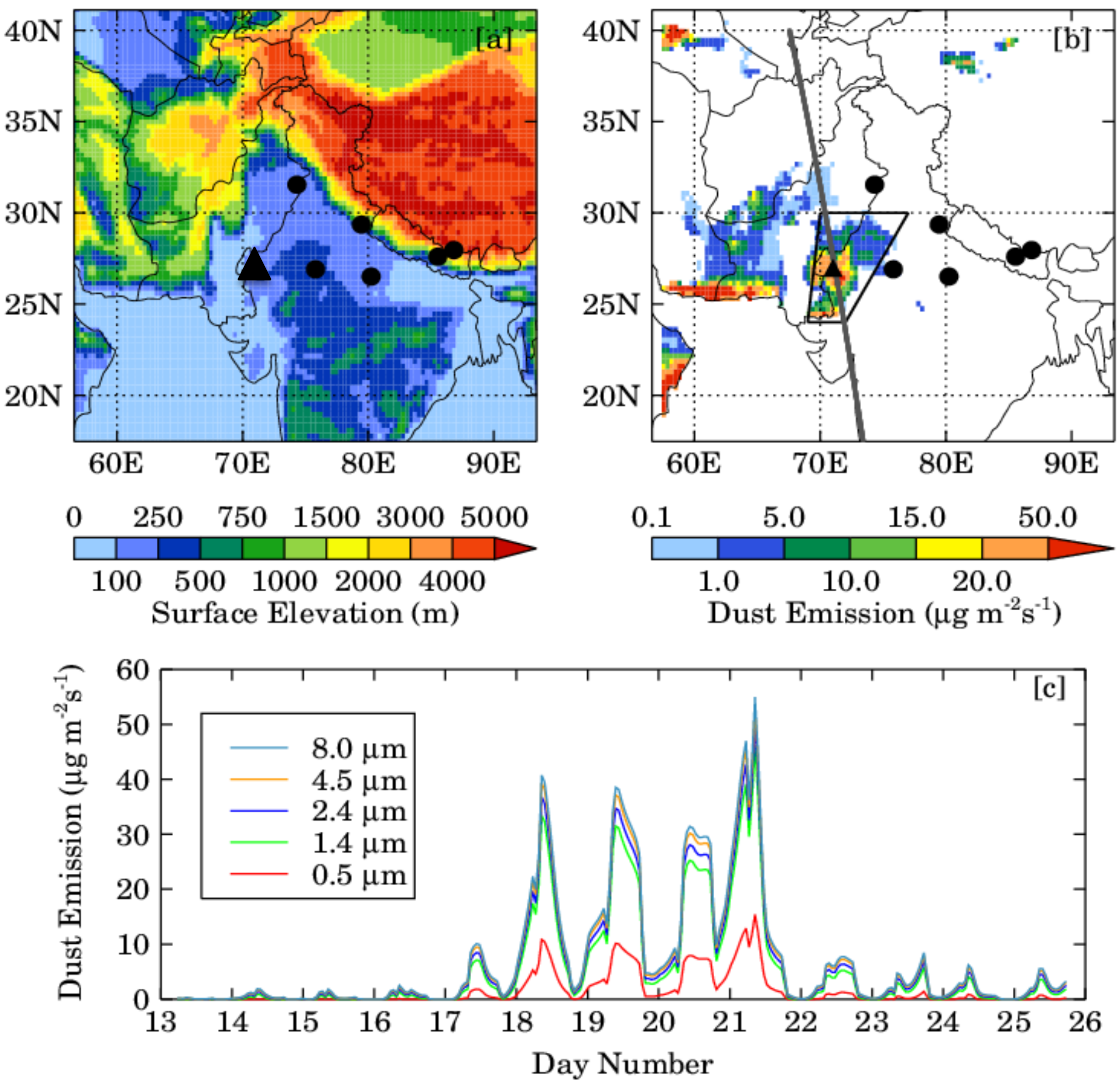
What time step is used?

Courant-Friedrichs-Levy Condition says to maintain stability the following must be met:

$$\left| \frac{u \ \Delta t}{\Delta x} \right| \leq 1$$

Sometimes (deep convection) *w* and Δz should be considered instead of u and Δx.

WRF-Chem set-up



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

Top of model: 10 hPa

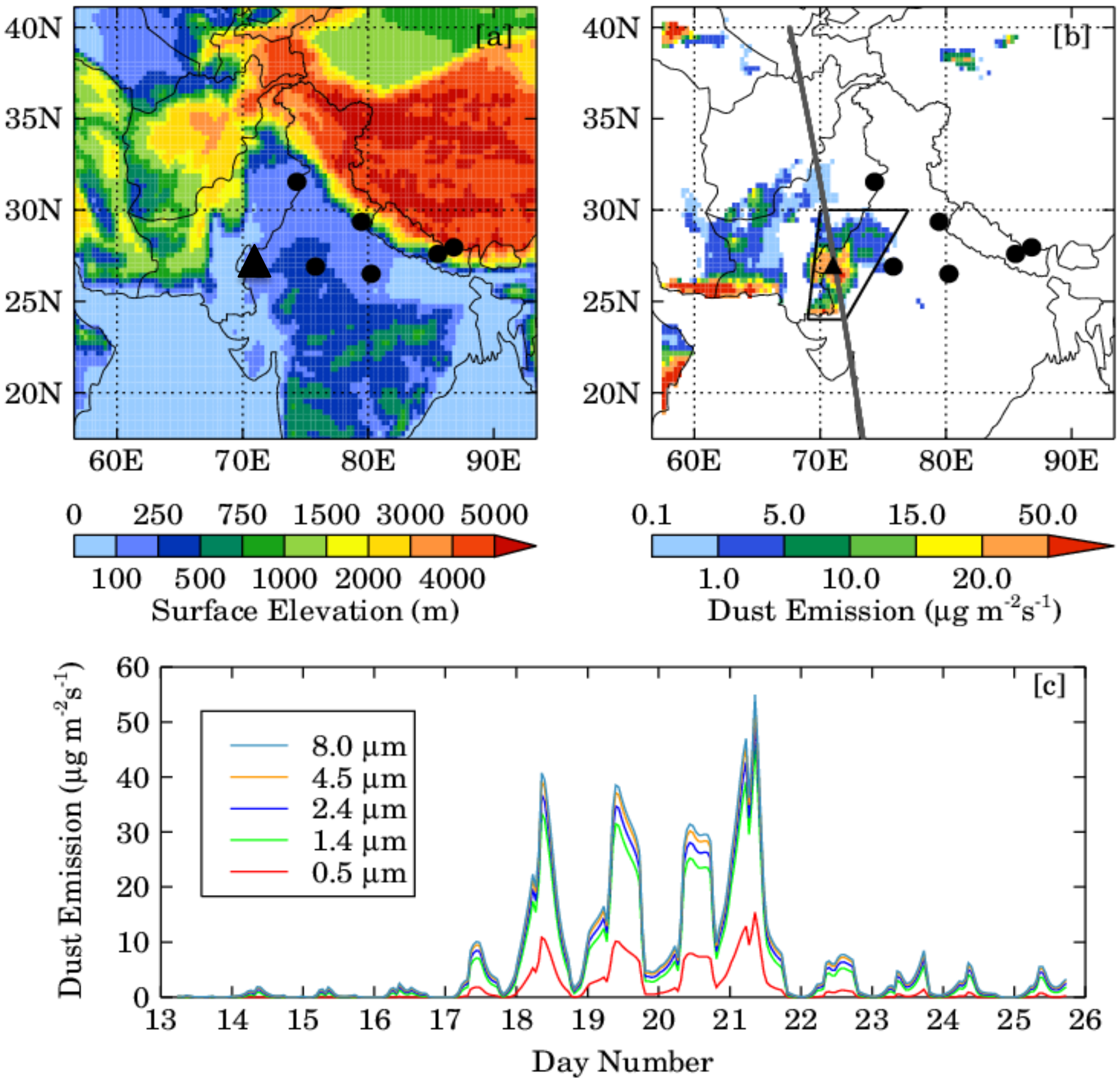
What time step is used?

To prevent instabilities in solving transport equations, time steps need to be small.

Rule of thumb:
Δt (seconds) = 6 Δx (km)

Δt = 120 seconds was used here

WRF-Chem set-up



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Grid points (x,y,z) = (120,90,51)

Simulation: 10-25 Apr 2010

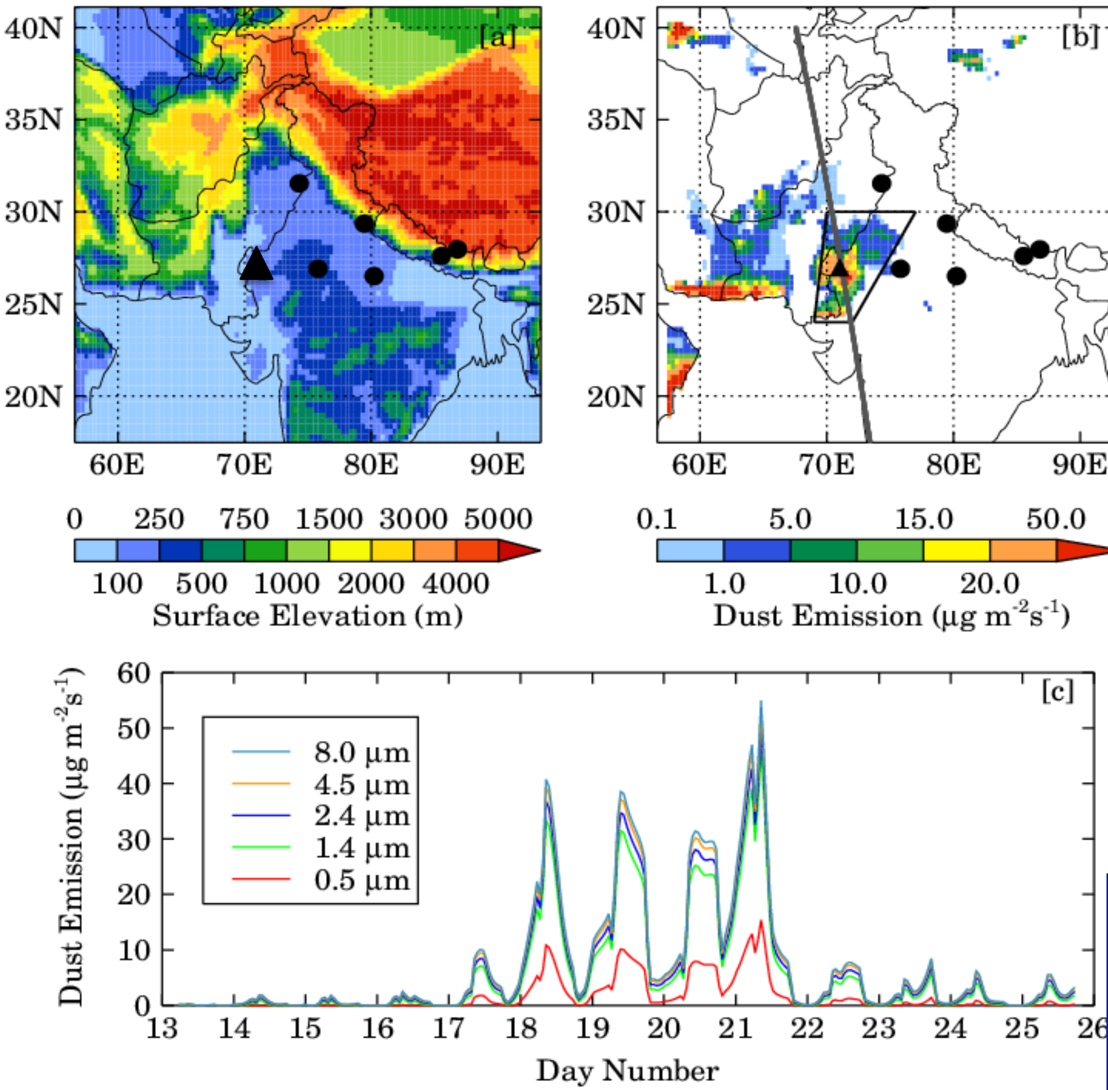
Δt = 120 seconds

Let's increase the resolution!

Δx = 15 km

How much more does it cost to run the simulation?

WRF-Chem set-up



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Simulation: 10-25 Apr 2010
Δt = 120 seconds

Let's increase the resolution!
Δx = 15 km

How much more does it cost to run the simulation?

2 nx × 2 ny = 4 times more grid points

6 Δx = 90 seconds
→ 5-8 times more including Δt change

Model Configuration for Dust Storm Simulation

1. **Transport**
2. Physics
3. Chemistry and Aerosol Representation
4. Aerosol Optical Properties

Model Configuration for Dust Storm Simulation

Atmospheric evolution of species X is given by the *continuity equation*

$$\frac{\partial [X]}{\partial t} = E_X - \nabla \bullet (\mathbf{U}[X]) + P_X - L_X - D_X$$

local change in concentration with time

emission

transport (flux divergence; U is wind vector)

chemical production and loss (depends on concentrations of other species)

deposition

This equation cannot be solved exactly ⇨ need to construct *model* (simplified representation of complex system)

Transport schemes vary! Some schemes may not ensure that trace gas and aerosol concentrations are greater than zero.
→ Use schemes that maintain positive concentrations

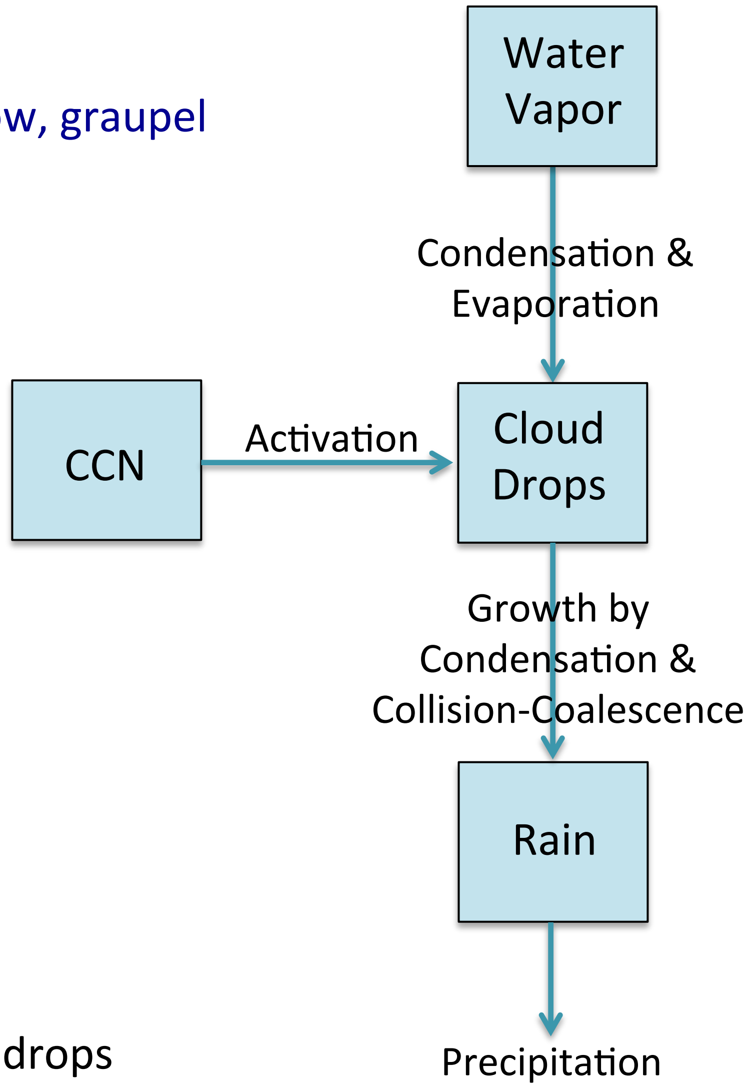
Model Configuration for Dust Storm Simulation

1. Transport
2. **Physics**
3. Chemistry and Aerosol Representation
4. Aerosol Optical Properties

WRF-Chem set-up

Cloud Physics:
Formation of cloud drops, rain, cloud ice, snow, graupel

Types of schemes:
1. Predict mass mixing ratio
2. Predict number and mass mixing ratio
3. Predict N, M, size of cloud particles



CCN = Cloud Condensation Nuclei
= aerosols that activate to become cloud drops

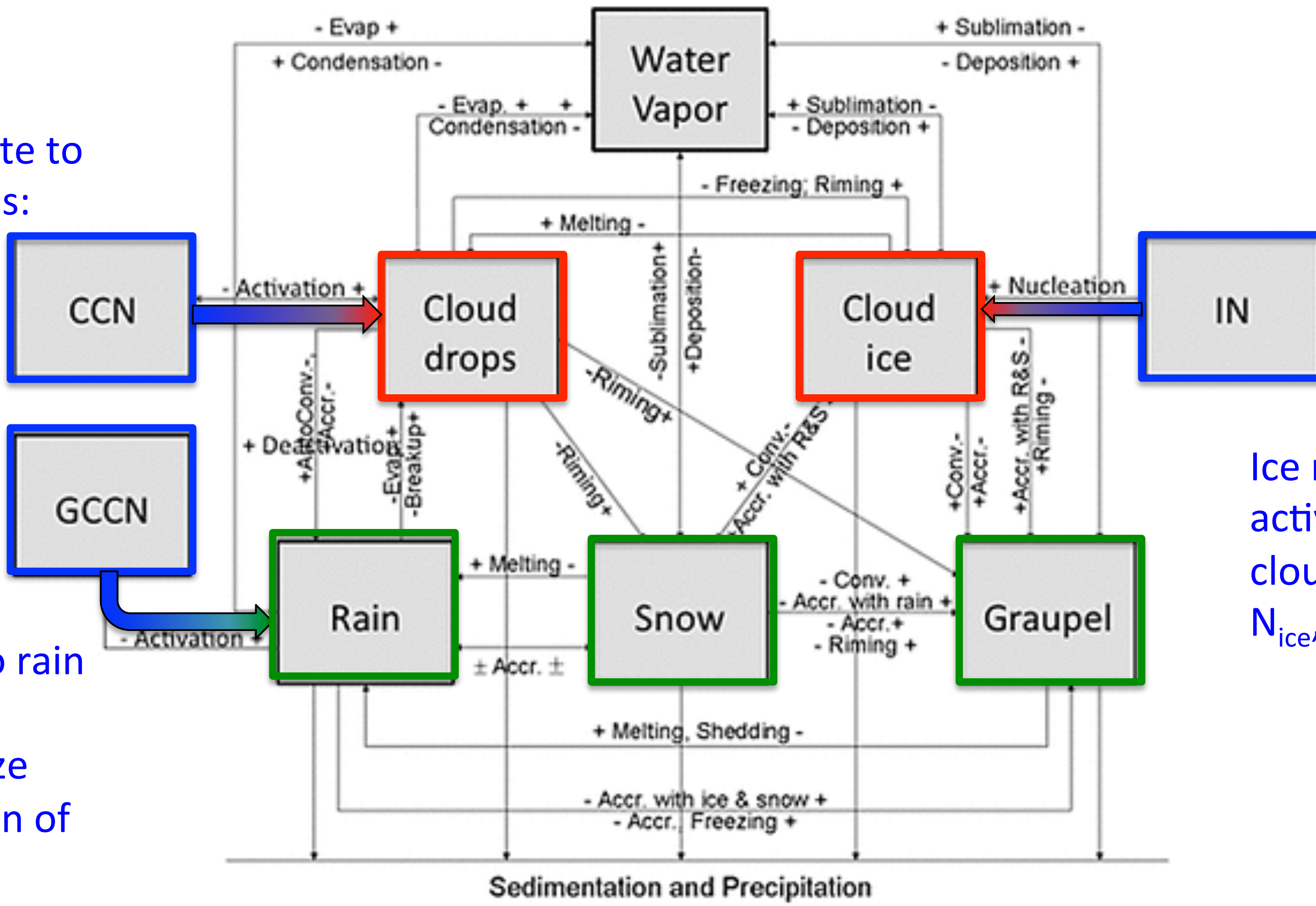
Graupel and Hail

Graupel forms when supercooled droplets of water are collected and frozen on falling snowflakes. Snow pellets are graupel.

Hail is solid precipitation, water ice. It has layers of water (from liquid drops and vapor) as its structure.

Predict N and M of aerosols and cloud particles

CCN activate to cloud drops: N_d, q_c



Giant CCN activate to rain drops: N_r from size distribution of q_r

Ice nuclei activate to cloud ice: N_{ice}, q_{ice}

Aerosols **Non-precipitating cloud hydrometeors**

Precipitating cloud hydrometeors

N = number
M = mass
CCN = cloud condensation nuclei
q = mass mixing ratio

WRF-Chem set-up

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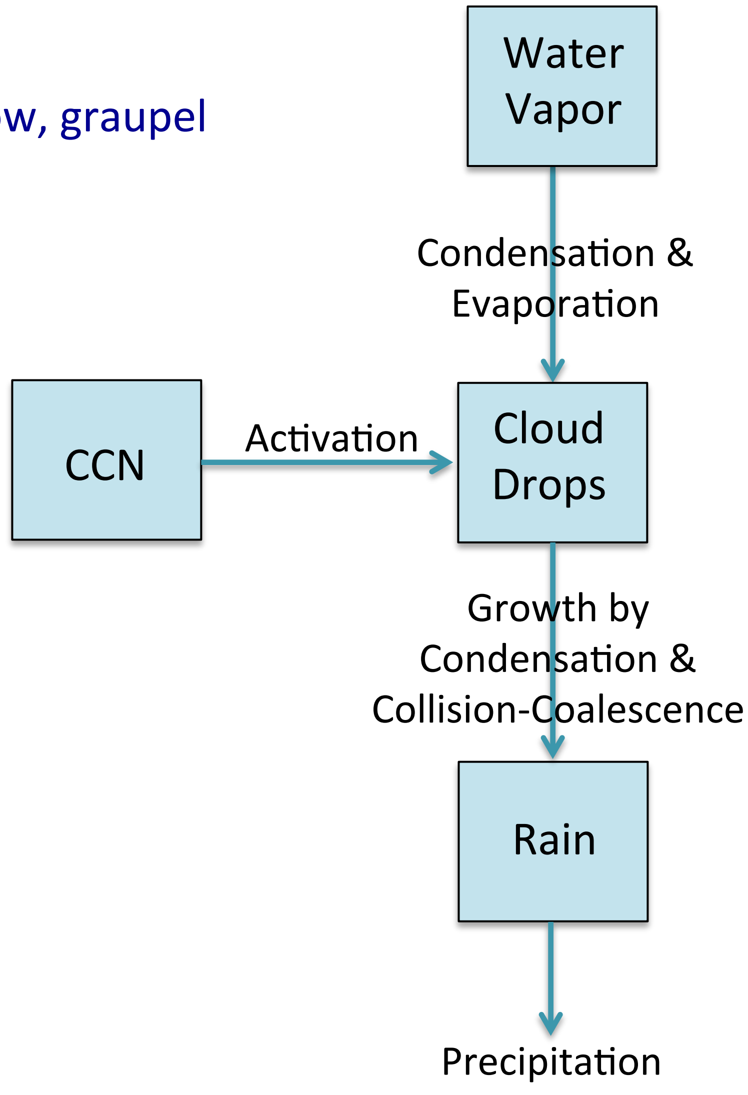
2. Predict number and mass mixing ratio
3. Predict N, M, size of cloud particles



Which scheme do you use?

WRF-Chem set-up

Cloud Physics:
Formation of cloud drops, rain, cloud ice, snow, graupel
(Thompson scheme was used)

Cumulus Parameterization:
Transport in convective clouds that cannot be done by vertical velocity
(Kain-Fritsch scheme was used)

Surface and PBL:
Transport in boundary layer that cannot be done by u, v, w
(MYJ scheme was used)

Radiation:
Solar and longwave radiation for heating
(RRTMG scheme was used)

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Which scheme do you use?

It is best to run WRF only trying different schemes to see which combination represents reality best. Note – nudging or data assimilation can help, especially if not focused on chemistry-meteorology interactions.

Model Configuration for Dust Storm Simulation

1. Transport
2. Physics
3. **Chemistry and Aerosol Representation**
4. Aerosol Optical Properties

Some Aerosol Representations

1. Kumar et al. (2014) Dust effects on radiation and aerosol optical properties
2. Kumar et al. (2014) Dust effects on chemistry

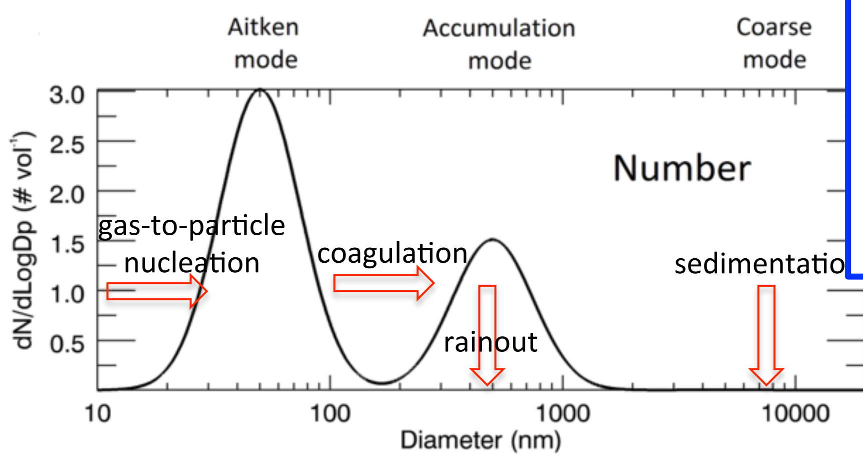
- Bulk mass mixing ratios
- Modal aerosol models
- Sectional bin models

In general:

Bulk models do not represent aerosol chemistry well (working on it, so it depends on current status of model)

Bulk models: sulfate, black carbon, organic carbon, dust (4-6 sizes), sea salt (4-6 sizes)

Modal and Sectional models predict mass and number → aerosol-cloud interactions are possible to study



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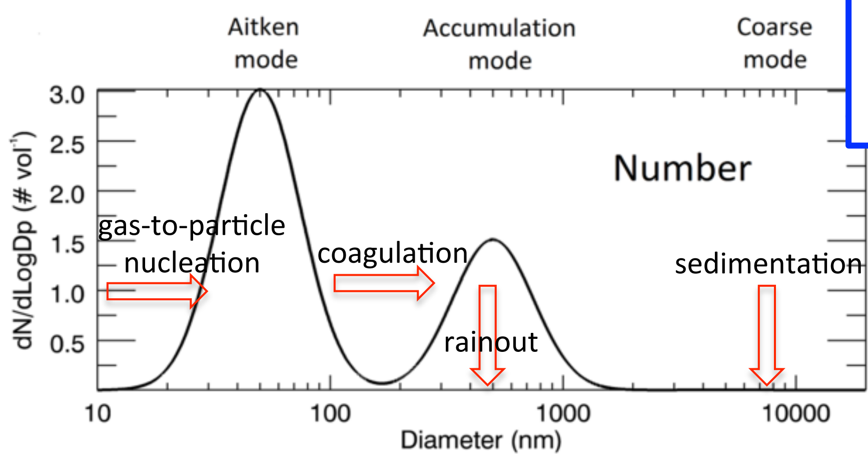

Which scheme do you use?

Bulk scheme great if focused only on trace gas chemistry.

Modal and Bin schemes for aerosol-cloud interactions

Some Gas-Phase Chemical Mechanisms

- SAPRC07 or SAPRC99
- RADM or RACM
- Carbon Bond (CBM5, CBMZ)
- MOZART
- U Manchester
- Reduce Hydrocarbon
- GEOS-Chem and many others

70-200 trace gases
100s of chemical reactions

What's the difference among these mechansims?

30 trace gases
68 chemical reactions

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100s of chemical reactions

What's the difference among these mechansims?

30 trace gases
68 chemical reactions

Which mechanism do you choose for your simulation?
Personal preference mostly. However, if forecasting (needing runs done quickly) use a mechanism with fewer trace gases. Most of the time is spent in the advection of all the trace gases and aerosols.

Some Gas-Phase Chemical Mechanisms

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- RADM or RACM
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100s of chemical reactions

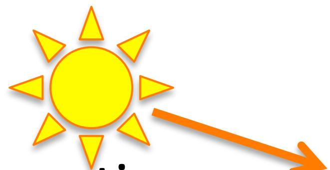
What's the difference among these mechansims?

30 trace gases
68 chemical reactions

Which mechanism do you choose for your simulation?

GOCART aerosol scheme, MOZART gas chemistry was used

Quantifying Photolysis Rates



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

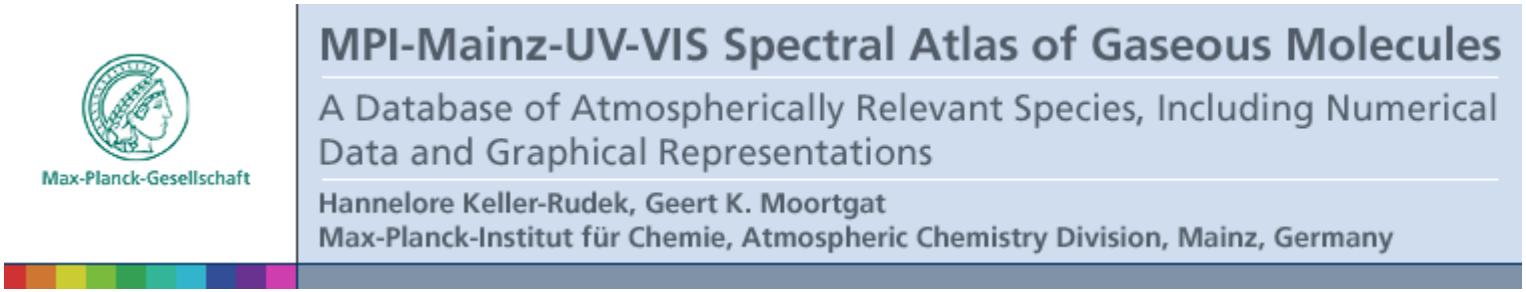
$F(\lambda) =$ spectral actinic flux, quanta $cm^{-2}\ s^{-1}\ nm^{-1}$

= solar radiation flux onto sphere

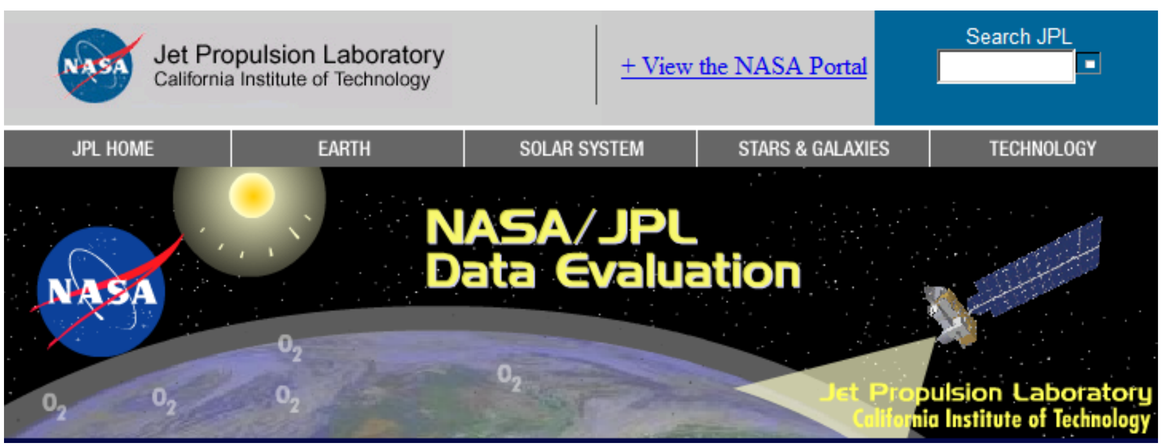
-- probability of photon near molecule

Compilations of Cross Sections & Quantum Yields

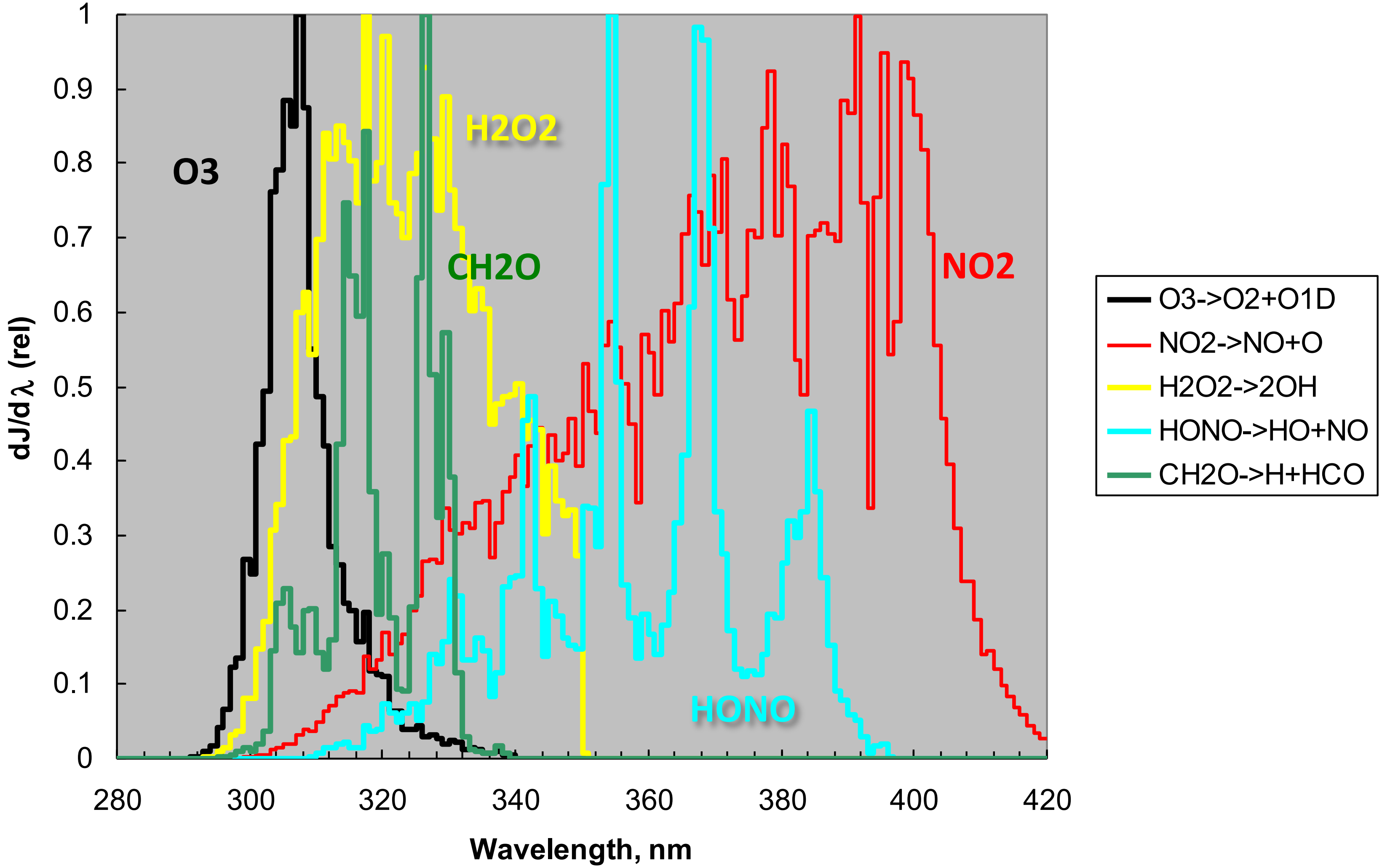
http://www.atmosphere.mpg.de/enid/2295



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



Photolysis Frequencies as Function of Wavelength



surface, overhead sun

Calculation of Photolysis Rates

1. Kumar et al. (2014) Dust effects on radiation and aerosol optical properties
2. Kumar et al. (2014) Dust effects on chemistry

Radiation calculation over the UV and into visible wavelengths

Detailed schemes (e.g. Troposphere Ultraviolet Visible (TUV) calculation)

Fast schemes (calculations at only a few wavelengths, e.g. Fast-J and F-TUV (fast TUV))

→ Need to be sure scheme accounts for clouds and aerosols!

F-TUV was used here

TUV website: http://cprm.acom.ucar.edu/Models/TUV/Interactive_TUV/

Emissions

- Anthropogenic Emissions
  - Several emissions inventories available
  - See ECCAD web site *eccad.sedoo.fr/*

Used here
MACCity emissions
FINN BB emissions used
MEGAN biogenic emissions

- Biomass Burning Emissions

GFED www.globalfiredata.org/

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

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

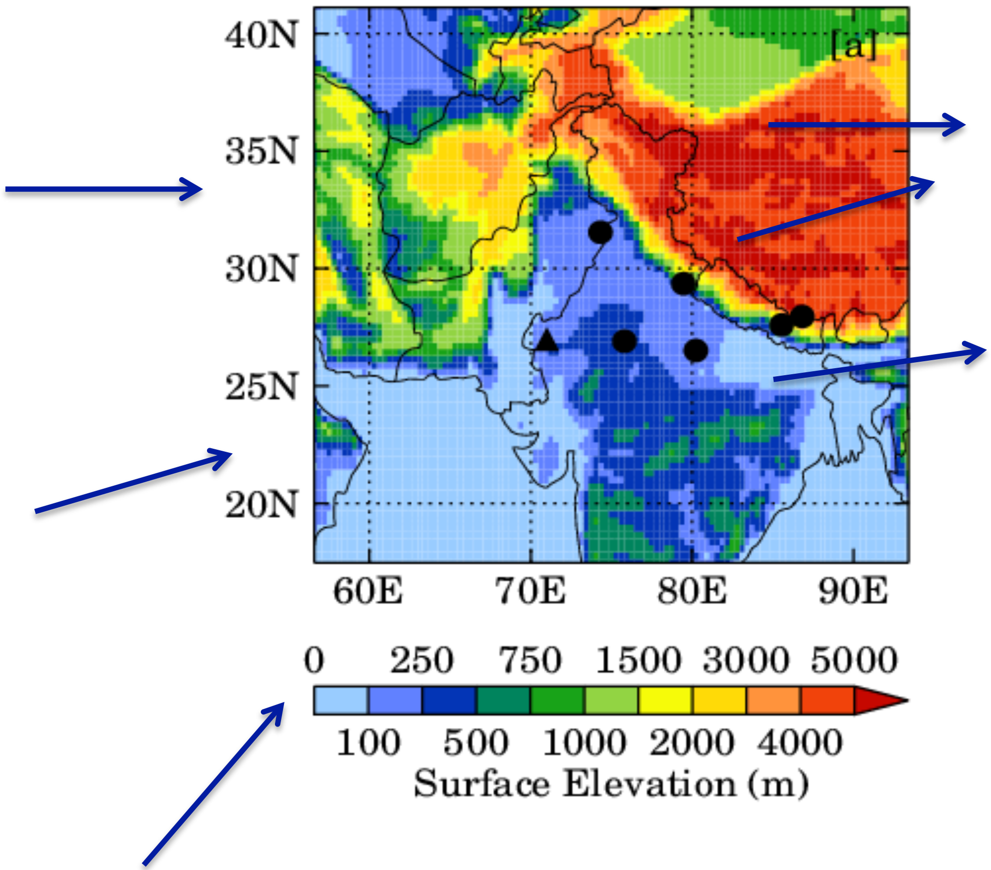
Forecast http://www.acom.ucar.edu/acresp/forecast/fire-emissions.shtml

- Biogenic Emissions

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

BEIS
https://www.epa.gov/air-emissions-modeling/biogenic-emission-inventory-system-beis

Initial and Boundary Conditions



Meteorology Variables:
Reanalysis products (ECMWF, NCEP, MERRA)

Chemistry Variables:
Global Chemistry Transport Models (CAM-Chem, GEOS-Chem, etc)

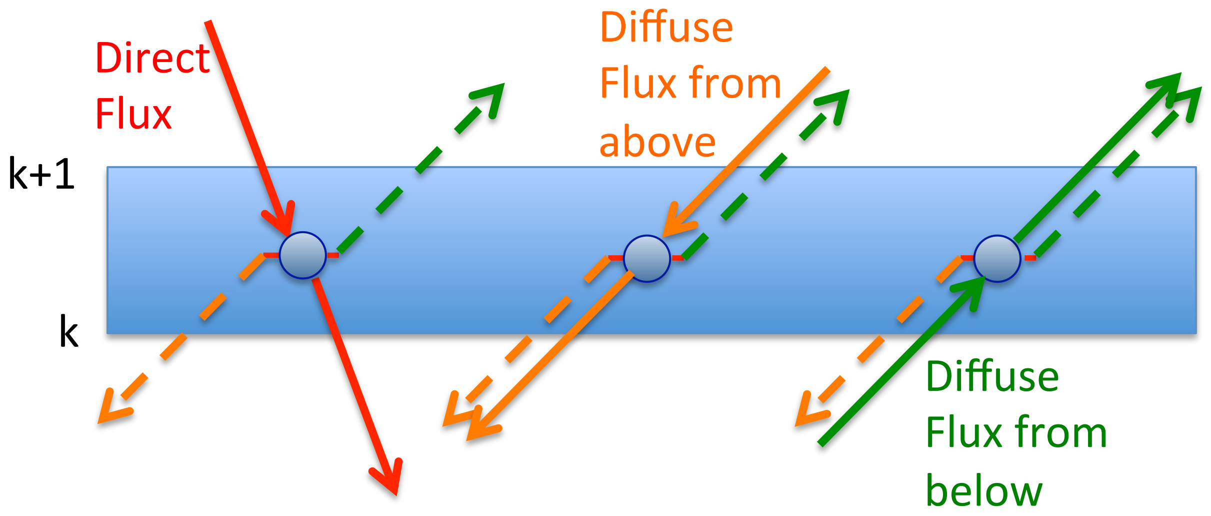
<u>Used here:</u>
NCEP FNL
MOZART-4 CTM

Model Configuration for Dust Storm Simulation

1. Transport
2. Physics
3. Chemistry and Aerosol Representation
4. **Aerosol Optical Properties**

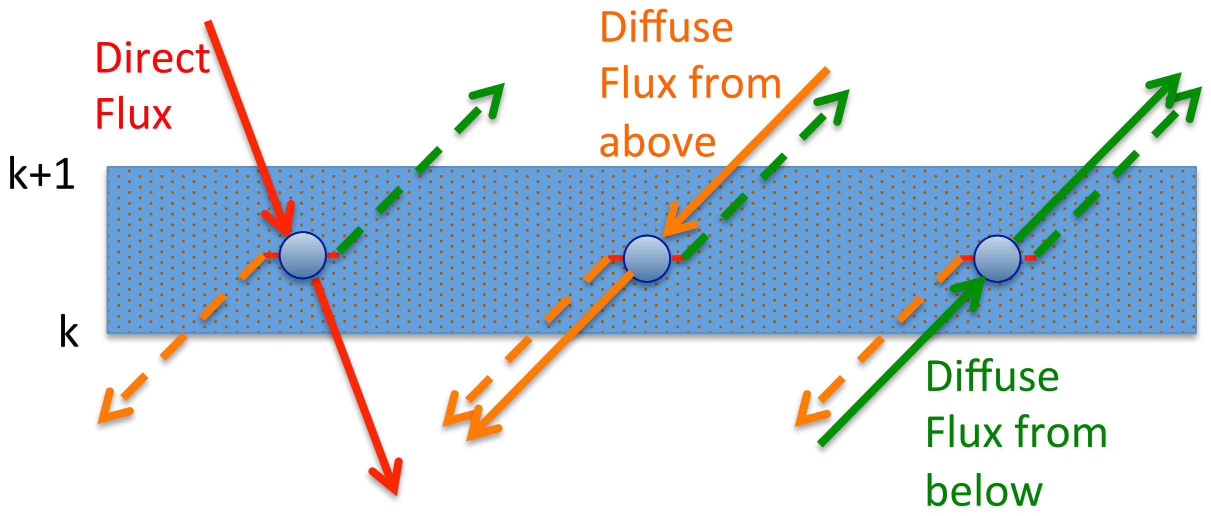
Aerosol Optical Properties

Need to do Radiative Transfer Calculations



Aerosols and Clouds Affect Radiation Flux

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, $f \sim (1+\mathbf{g})/2$

Used in dust simulation: aerosols are allowed to affect radiation

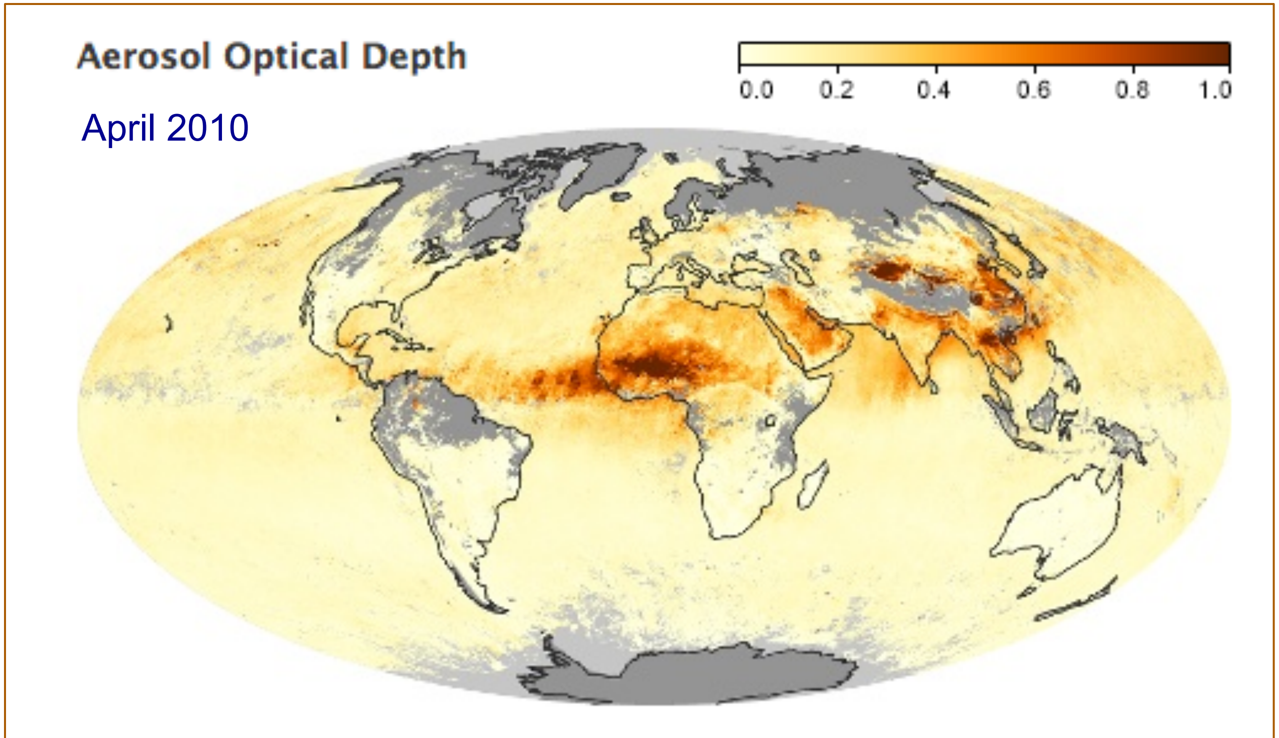
Aerosol Optical Depth (AOD)

- **Extinction coefficient**: fractional depletion of radiance per unit path length (km^{-1}) due to scattering and absorption by aerosols
- **Aerosol optical depth** (AOD) or **thickness** (AOT): integrated extinction coefficient over a vertical column, $I / I_o = e^{-AOD}$

AOD = 0 no aerosol effect

AOD ~ 1 "large"

AOD > 1 extremely high aerosol concentrations



Vertical optical depth

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

σ = attenuation cross section

n = number density of aerosols

z = altitude, λ = wavelength

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

Rayleigh scatt. $\sim 0.1 - 1.0$

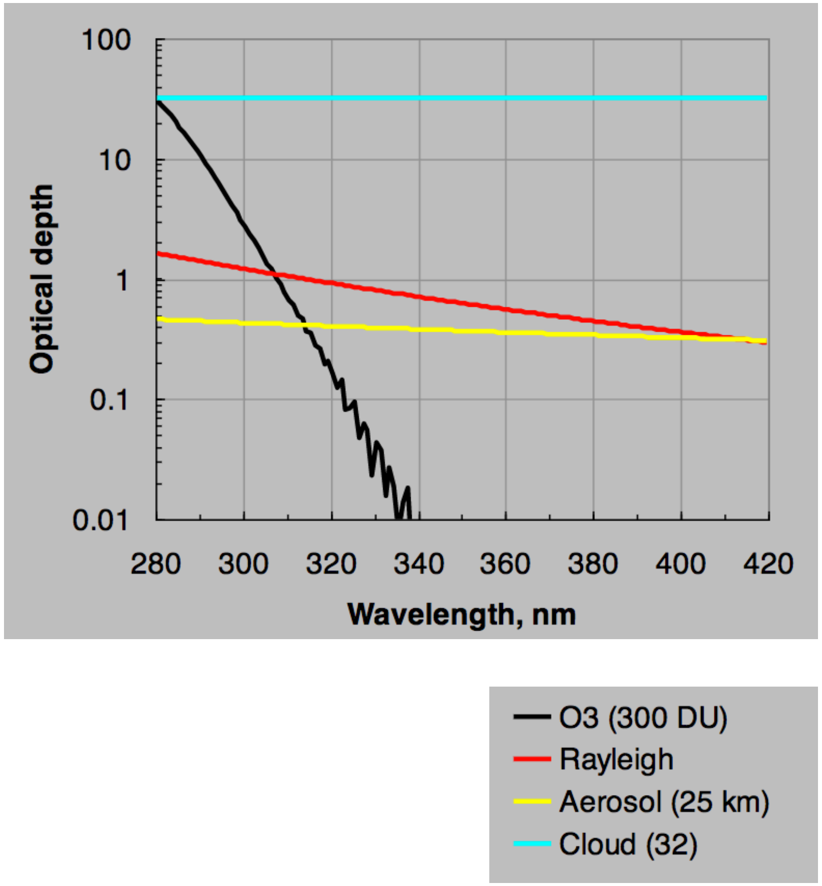
O_3 absorption $\sim 0 - 30$

for aerosols: $0.01 - 5.0$

for clouds: $1\text{-}1000$

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

cumulonimbus $\sim > 100$



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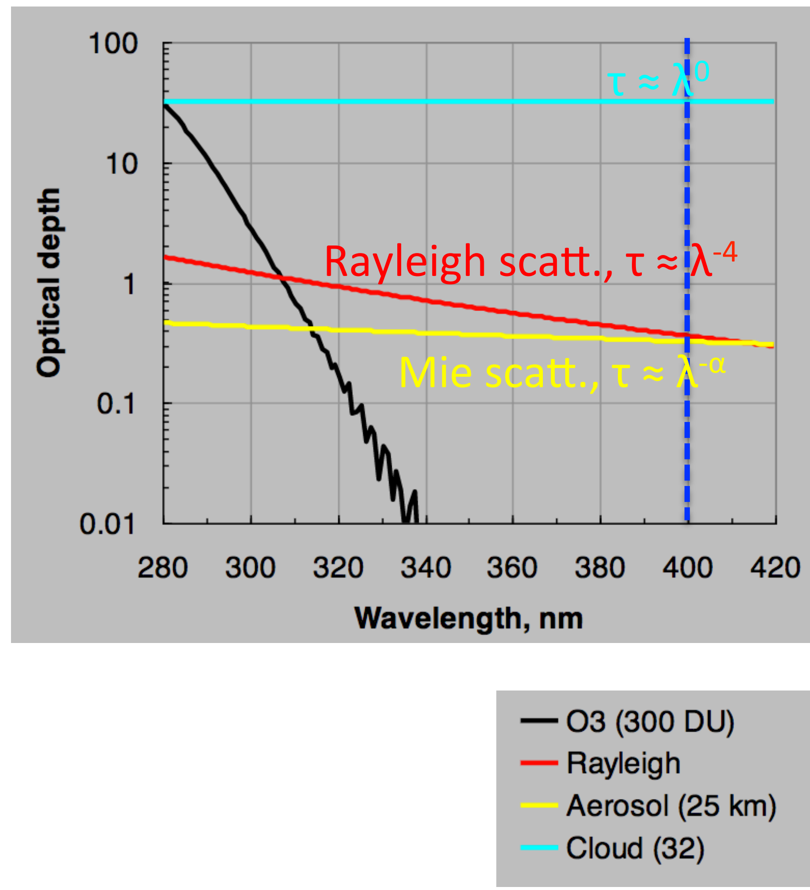

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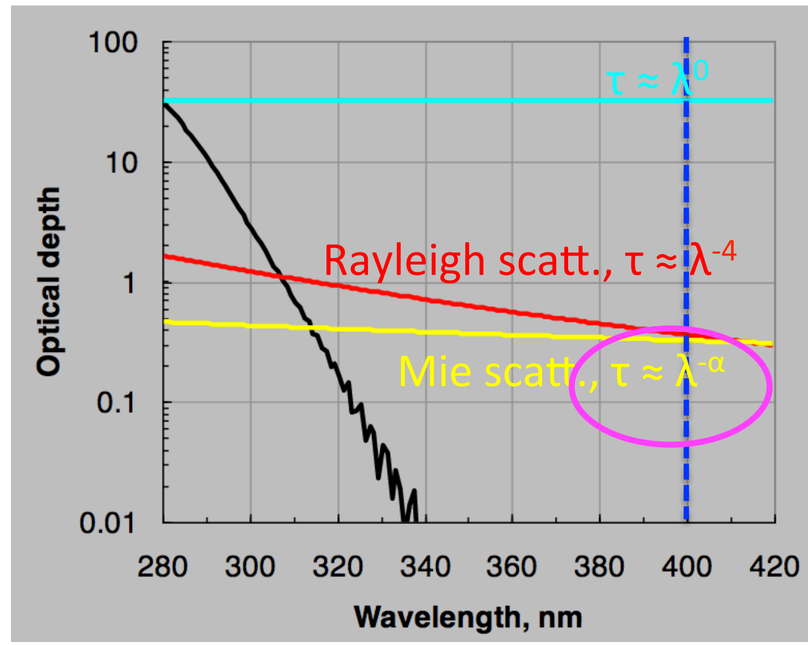
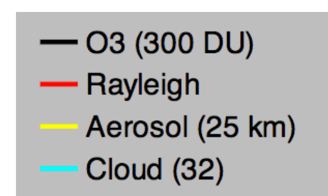


α = Ångström exponent



Aerosol optical depth

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

σ = attenuation cross section

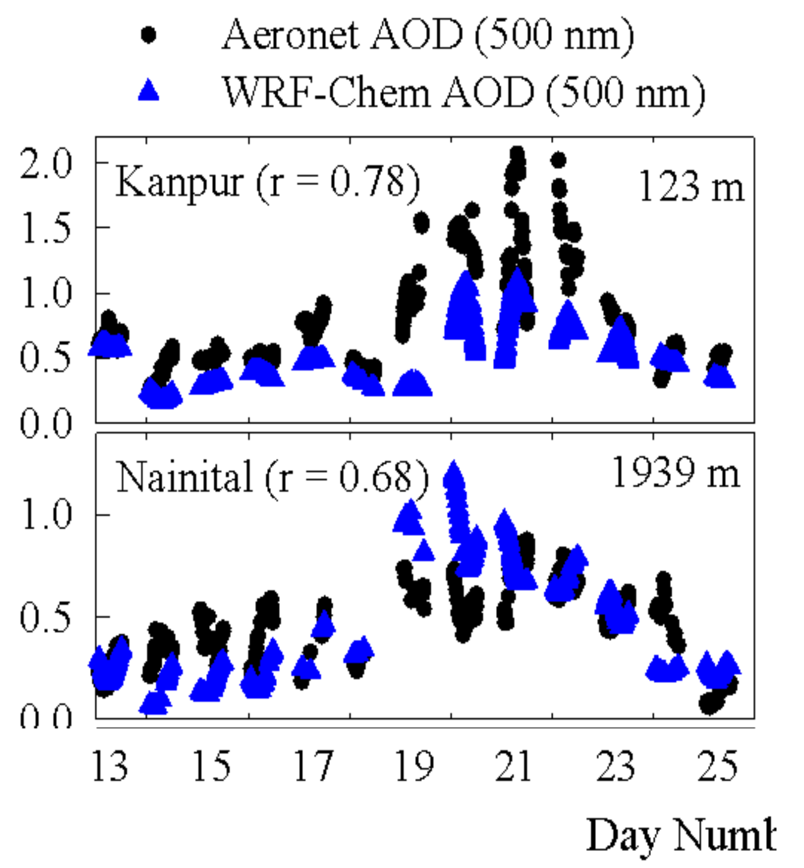
n = number density of aerosols

z = altitude, λ = wavelength

for aerosols: 0.01 - 5.0

Dust storm case gives

AOD of 1.0 – 2.0 at λ = 500 nm



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, SSA is strongly λ-dependent

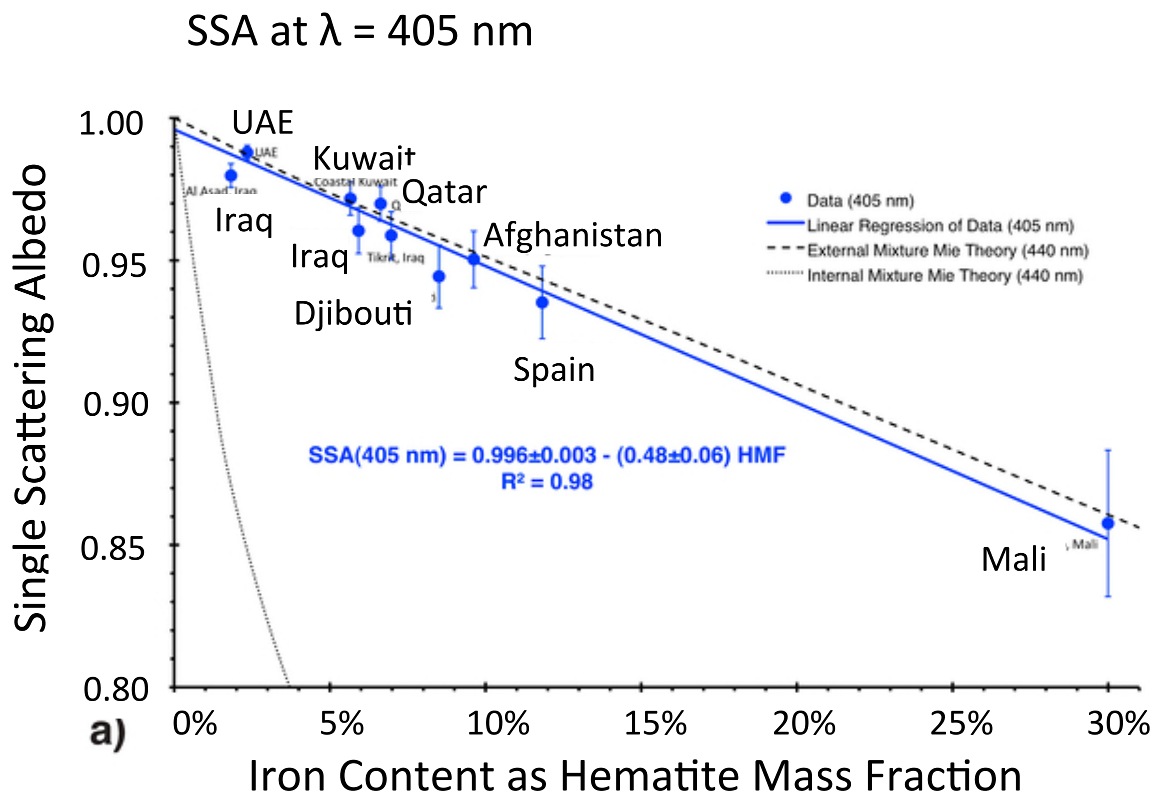
for aerosols:

sulfate ~ 0.99

soot, organics ~ 0.8 or less,

SSA can vary for dust

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



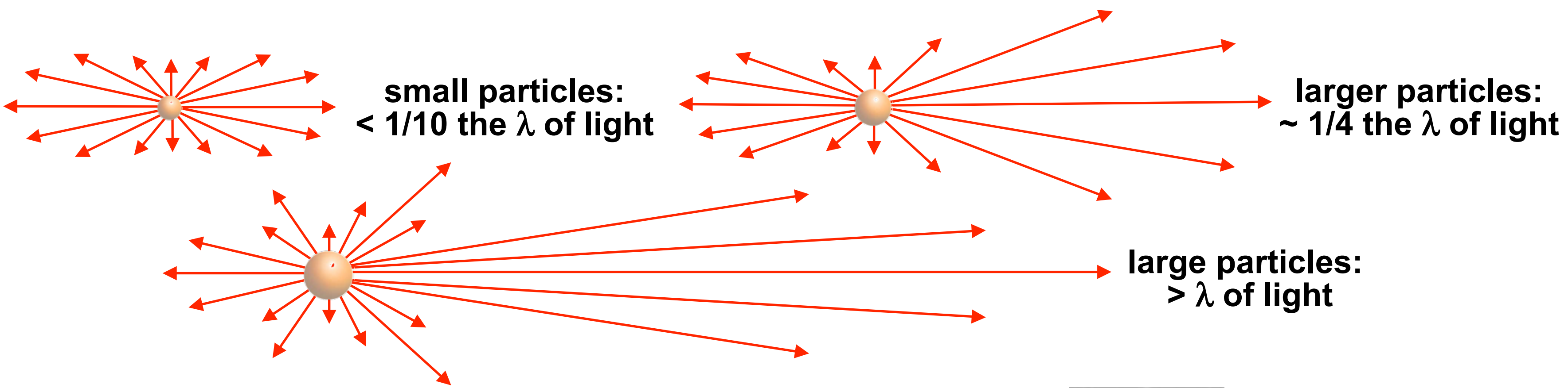
Moosmuller et al. (2012)
Journal of Geophysical Research: Atmospheres
Volume 117, Issue D11, D11210, 8 JUN 2012 DOI: 10.1029/2011JD016909
http://onlinelibrary.wiley.com/doi/10.1029/2011JD016909/full#jgrd17711-fig-0003

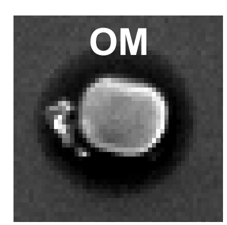
Asymmetry factor, $g(\lambda, z)$

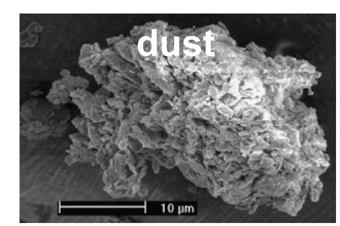
Preferred scattering direction for the light encountering the aerosol particles

- range -1 to + 1
  - pure back-scattering = -1
  - isotropic or Rayleigh = 0
  - pure forward scattering = +1
- depends on size and composition of aerosols
  - for aerosols:, typically 0.5-0.7
  - for clouds, typically 0.7-0.9

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

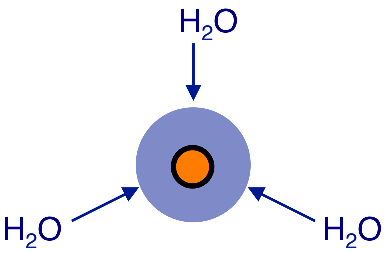






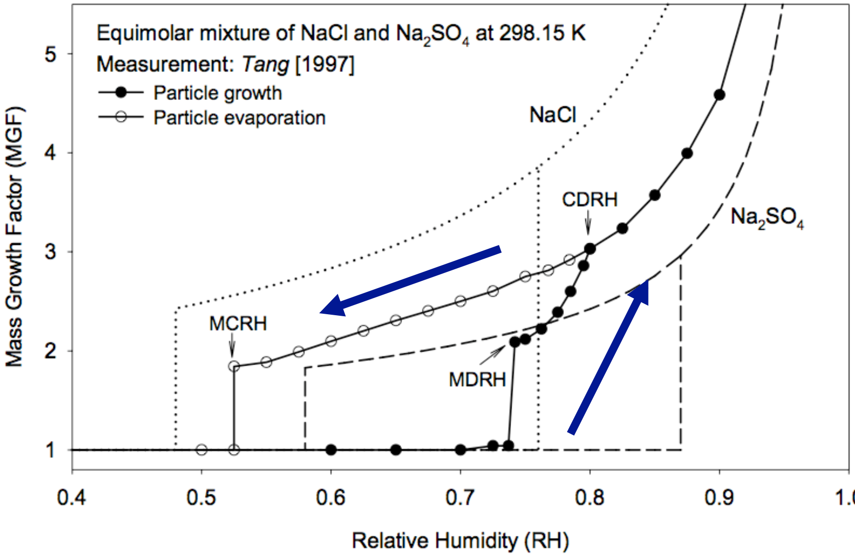
Importance of Aerosol Water

- Aerosol water will have a big impact on optical properties



- Uptake of water by aerosols depends on relative humidity (RH); predictions of RH need to be examined when evaluating aerosol direct radiative effects

► Composition affects water uptake: hydrophobic vs. hydrophilic aerosols



Refractive Indices

- Refractive index of a substance is a dimensionless number that describes how light propagates through a medium
- Refractive indices in models based on literature values derived from laboratory experiments, vary with wavelength for some aerosol compositions

Default Values for SW Radiation in WRF (users can change)

	real part		imaginary part
BC =	1.850	+	0.71i (all λ)
OM =	1.450	+	0.00i (all λ)
SO_4 =	1.468	+	1.0e-9i (300 nm), small λ dependence
NH_4NO_3 =	1.500	+	0.00i (all λ)
NaCl =	1.510	+	0.866e-6i (300 nm), small λ dependence
dust =	1.550	+	0.003i (all λ), depends on type of dust
H_2O =	1.350	+	1.52e-8i (300 nm), small λ dependence

↳ greater the # ➡ more absorption

similar relationships for LW radiation

WRF Methodology for Calculating Aerosol Optical Properties

Generic Aerosol Optical Property Module

size and number distribution
composition
aerosol water
→ refractive indices → Mie theory → layer optical depth, AOD_l; single scattering albedo, w_o; asymmetry factor, g → shortwave / longwave radiation

- In WRF-Chem, AOD, ω_o, and g computed at
  4 wavelengths (**300, 400, 600, 1000** nm) for shortwave radiation
  16 wavelengths for longwave radiation

Ångström exponent used to convert to wavelengths needed by radiation schemes

Ångström exponent:

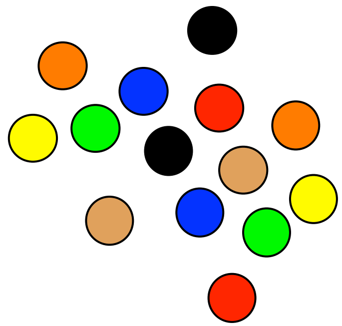
$$\alpha = -\frac{\log \frac{\tau_{\lambda_1}}{\tau_{\lambda_2}}}{\log \frac{\lambda_1}{\lambda_2}}$$

To compare WRF output to AERONET observations, must convert AOD to λ=550 nm using this Ångström exponent equation

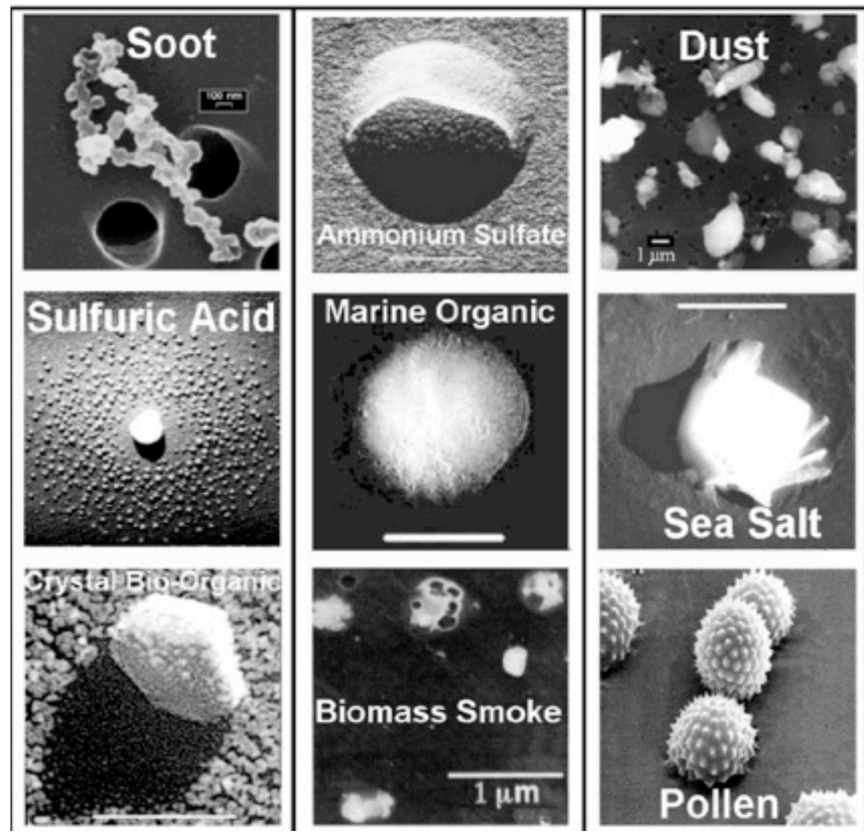
$$\tau(\lambda) = \tau(400nm) \times \left(\frac{\lambda}{400}\right)^{-\alpha}$$

Aerosol Mixtures

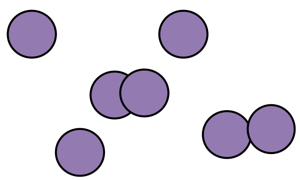
External Mixture:
Each particle is separate in composition: BC, sulfate, sea salt



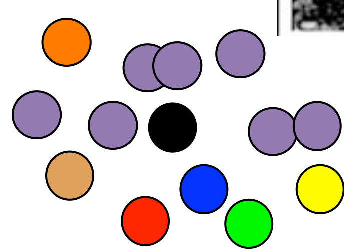
No combinations, e.g. sulfate coating BC aerosol



Internal Mixture:
Each particle is same composition: BC+sulfate+sea salt



Reality:
Have aerosols that are both external and internal mixtures

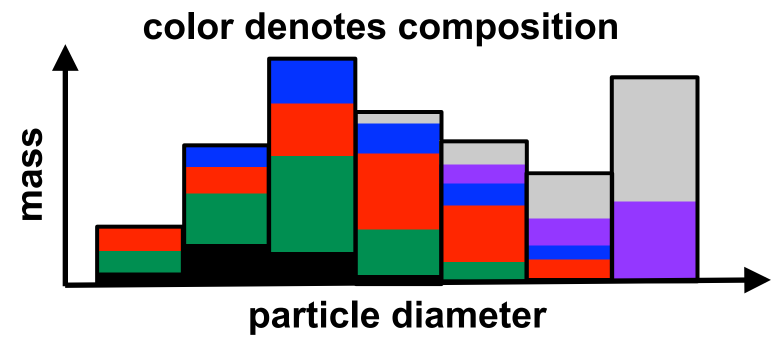


Aerosol composition is important in affecting radiation – extent of scattering vs absorbing

Mixing Rules for Mie Calculations

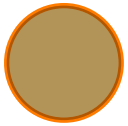
Refractive indices need to be averaged among the compositions in some way for discrete size ranges of the aerosol size distribution.

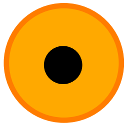
All particles within a size range assumed to have the same composition, although relative fraction can differ among size ranges.



Currently three choices in WRF-Chem:

- **Volume Averaging:** averaging of refractive indices based on composition
- **Shell-Core**: black carbon core and average of other compositions in shell (Ackermann and Toon, 1983; Borhren and Huffman, 1983)
- **Maxwell-Garnett:** small spherical randomly distributed black carbon cores in particle (Borhren and Huffman, 1983)





Used in dust simulation: volume averaging method

Concluding Comments on Configuring Chemistry Transport Models

- What is your goal of the simulation?
- What phenomena are you simulating?
  - Clouds? Mesoscale? Cloud scale?
  - Air quality of urban neighborhood? of Indo Gangetic Plain?
- What size domain is appropriate?
  - Should be big enough such that values at boundaries of domain do not affect the analysis of model results
- Are there special diagnostics needed?
  - PBL height? Aerosol optical depth? Chemistry production of ozone?

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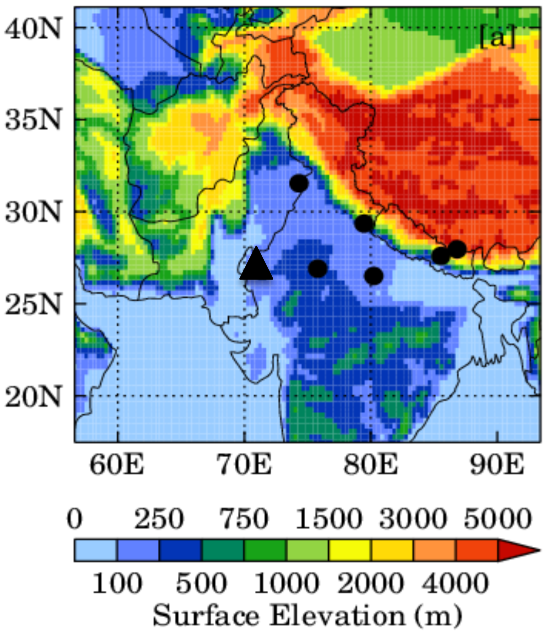
Questions?

Exercise



MAGIC, MEAT, AC[2]I[2]GP field campaigns

What forecasts do you want for your field experiment? Weather forecasts? CO plume forecasts? Emission plumes? Ozone forecasts?

- What parameters are needed?
- What model configuration for the forecasts?

After field campaign

- What parameters to predict and analyze?
- What model configuration is best?