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# Data assimilation using optimal interpolation: Correcting chemical transport model predictions with satellite observations

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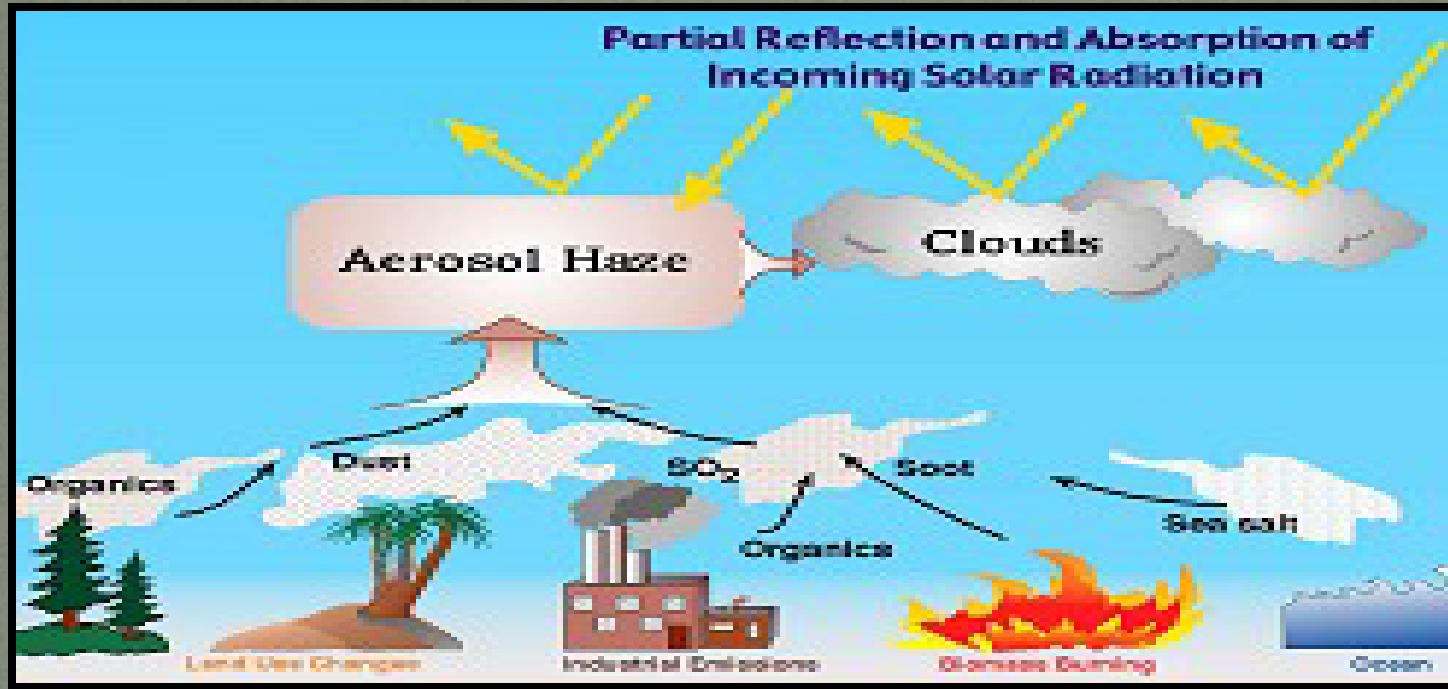
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# Introduction

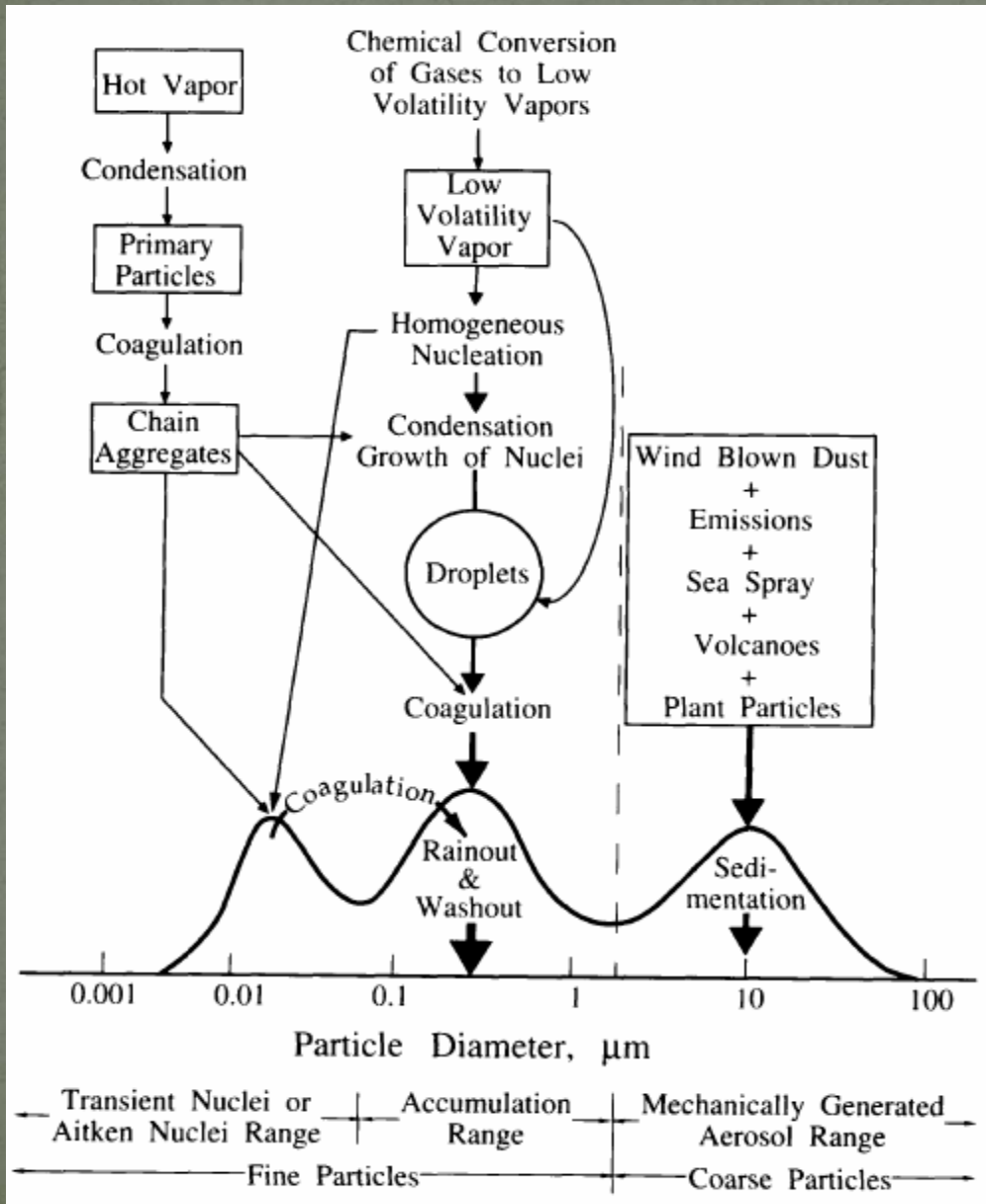


## Impact of anthropogenic aerosols on climate change

❑ **Perturbation of radiation balance** : scattering aerosols (sulphate, organic carbon, ions/water) reflect radiation, while absorbing aerosols (black carbon, BC) absorb and re-radiate thermal energy. Net cooling of Earth's surface, but heating of atmospheric layers with BC

❑ **Alteration of cloud properties and Hydrological cycle**

# Atmospheric processes affecting aerosols



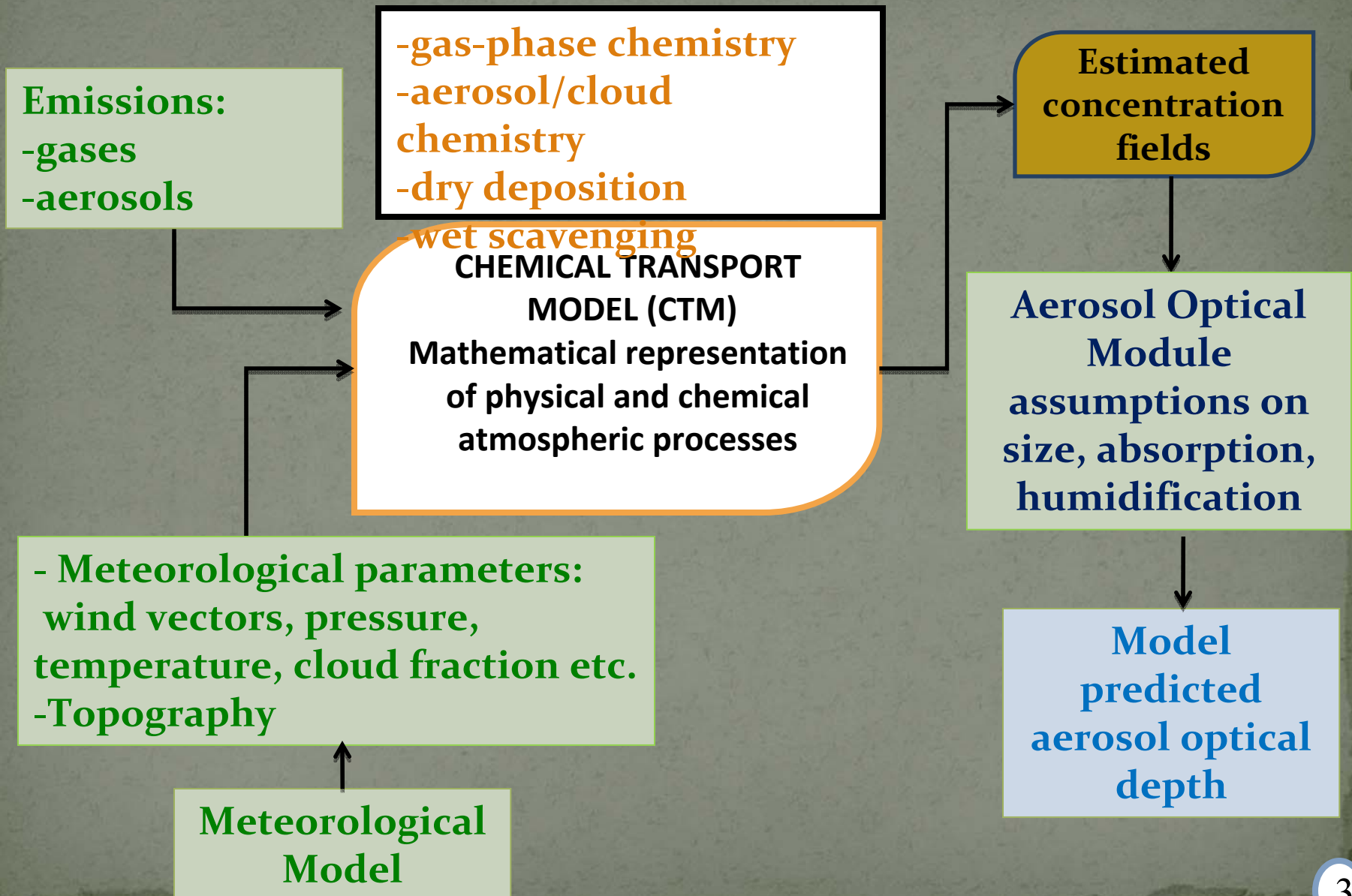
Microphysical processes :  
nucleation, coagulation, gas-to-particle conversion

Loss processes: dry deposition  
and wet scavenging

Interaction with clouds: cloud  
drop nucleation



# Chemical transport model



# Optical extinction properties

The change in radiation flux is given by:

$$\frac{-dI}{I} = \int_0^{TOA} \left[ \int_0^{\infty} \left( \frac{\pi d_p^2}{4} \right) K_{ext} \left( \frac{\pi d_p}{\lambda}, m \right) n(d_p) d(d_p) \right] dz$$

$n(d_p)$ , the particle number distribution,  $f(RH)$ , #  $m^{-3} \mu m^{-1}$

$K_{ext}$ , the extinction efficiency

$\lambda$ , the radiation wavelength, nm

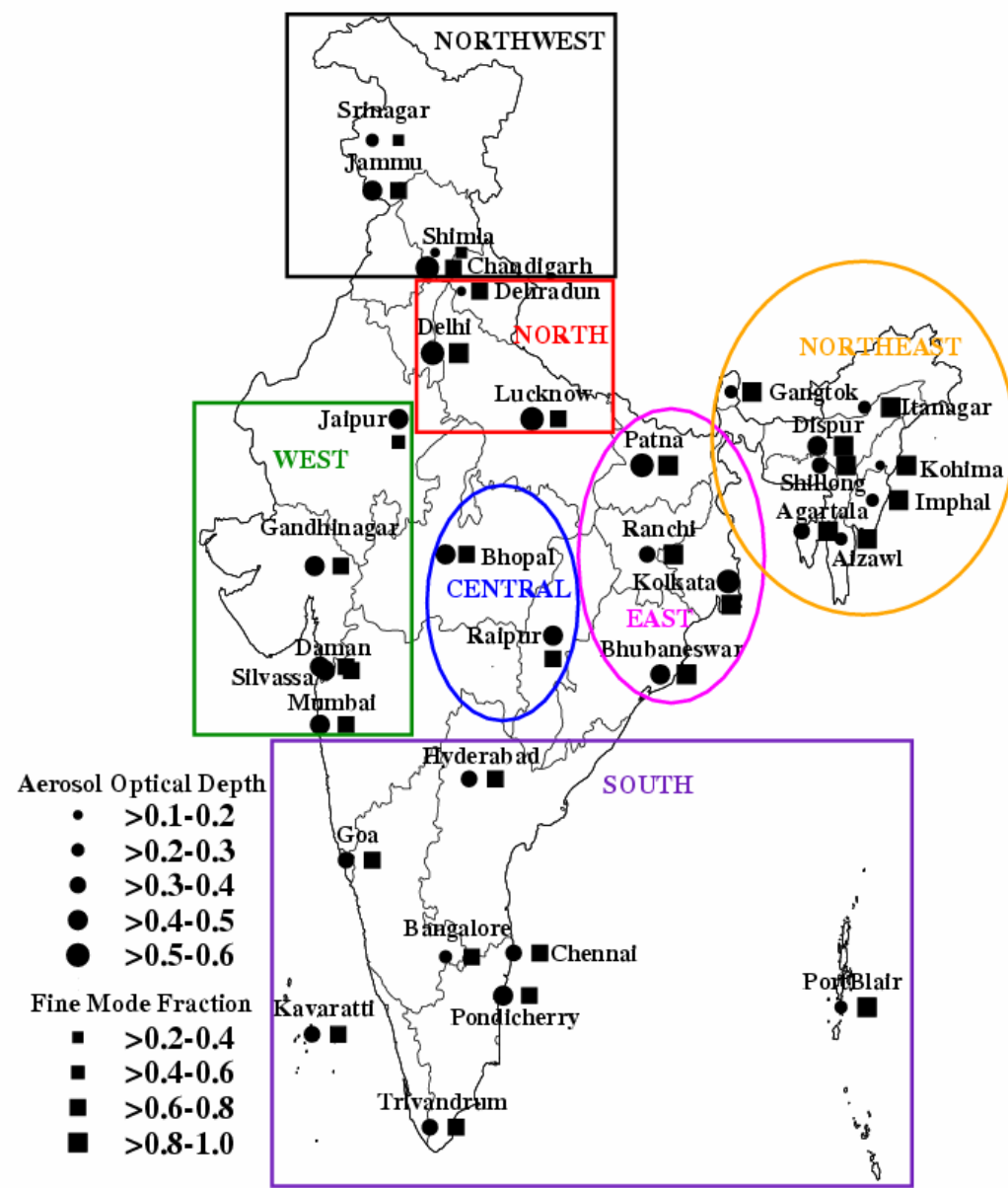
$m$ , the particle refractive index, real number for pure scatterers (sulphate) and imaginary number for absorbers (soot),  $f(RH)$ .

AOD, aerosol optical depth, term on the RHS

## Externally mixed aerosol model:

Assumed that aerosols are ensembles of pure particles (soot, sulphate, organic carbon, etc.) and the optical depth from each species is additive.

# Spatial and temporal aerosol heterogeneity



MODIS retrievals of aerosol optical depth (AOD) and fine mode fraction (FMF) have a regional character

Similar AODs but varying FMFs - Central India

Varying AODs and similar FMFs - Northeast

Varying AODs and FMFs - South India



Sources influencing columnar aerosols differ seasonally



# Need for data assimilation

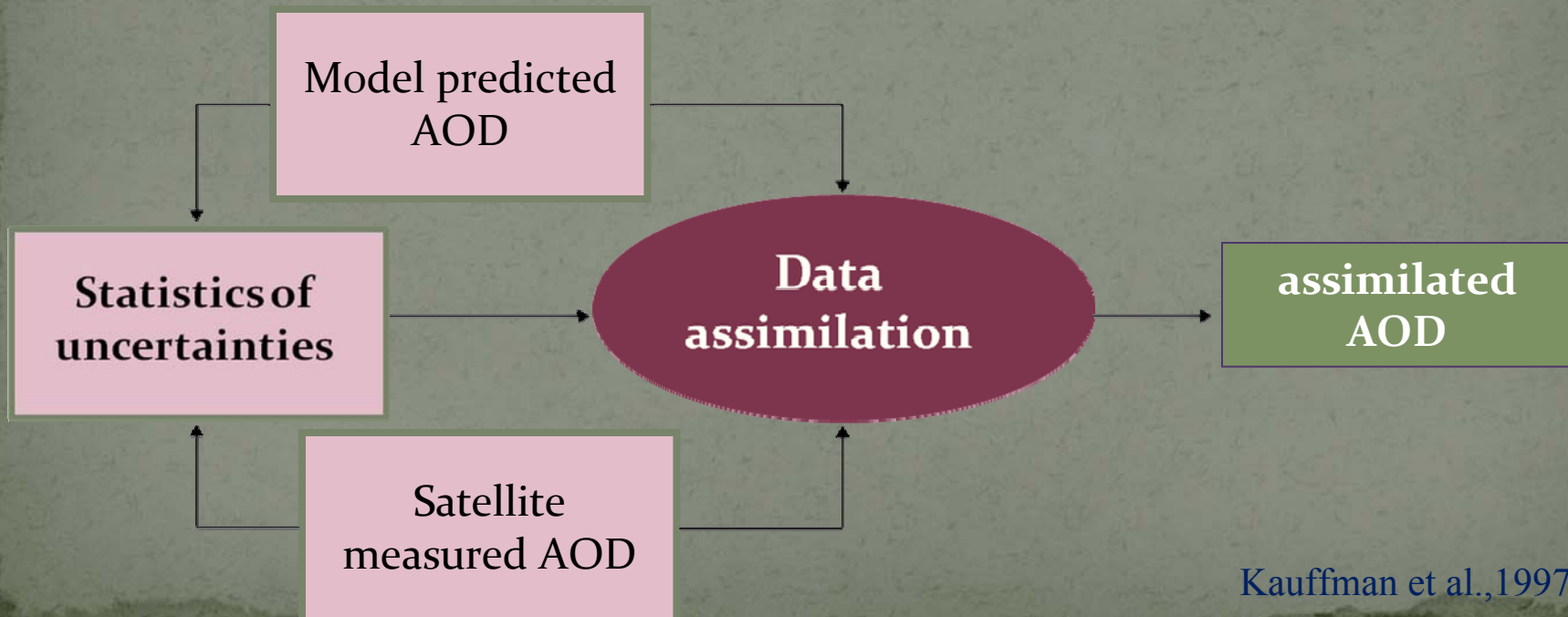
- ❑ Uncertainty in model predictions: emission magnitudes / spatial distribution, bias in model processes like chemistry or transport, simplified representation of sub-grid processes.
- ❑ Regional models typically under-predict both surface concentrations and AOD.
- ❑ Data assimilation (with satellite observations) has helped correct some of these errors (Collins et al. 2001; Adhikary et al. 2008; Chung et al., 2010)

However, persisting problems include:

- Quality of satellite data used.
- Accounting for uncertainty in observations.
- Accounting for uncertainty in model predictions.

# Framework for data assimilation

- ❑ Aerosol retrieval accuracy improved owing to advancement in satellite-based remote sensing. Advent of new and more sensitive instruments like the Moderate Resolution Imaging Spectroradiometer (MODIS)
- ❑ To improve the predictive capabilities of CTMs, they must be better constrained through the use of observational data.
- ❑ Data assimilation : statistical estimation method to reduce the uncertainty in the model parameter using model simulations(predictions), observations, and their respective statistics for errors.





# Objectives

**Aerosol data assimilation of predictions from a chemical transport model using satellite measurements of aerosol optical depth over south Asia.**

- ☐ Developing an algorithm to map the measurements by satellite onto model domain with weighting of different quality data.
- ☐ Improving an assimilation algorithm by better accounting for satellite measurement uncertainties.

# STEM-2K1(Sulfur Transport and dEposition Model)

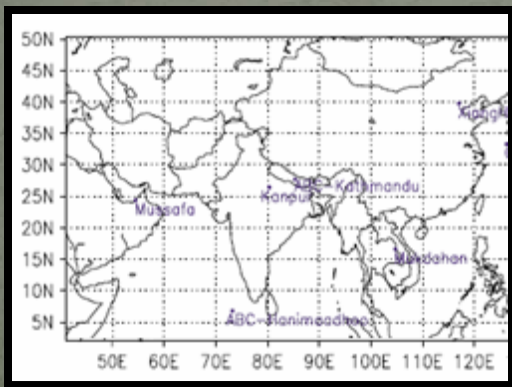
Has been successfully used in the past to study the seasonal cycle and outflow of aerosols from South and East Asia.

Model predicted species: sulfate, black carbon (BC), organic carbon (OC), sea salt and mineral dust.

Model resolution: 50 km x 50 km with 31 vertical layers extending up to 10hPa

For **sample case of March 2001**, model domain range : 5N to 45N latitude and from 40E to 120E longitude.

Meteorological parameters input: model WRF (Weather Research Forecasting)



Anthropogenic emissions inventory: inventory developed for TRACE-P intensive field campaign(Streets et al., 2003).

Dust and sea-salt emissions were calculated on-line using WRF meteorology.

Model domain (March 2001)

Carmichael et al. 2003, Adhikary et al. 2007 Chung et al. 2010



# Satellite data specifications

Moderate Resolution Imaging Spectroradiometer (MODIS) aerosol optical depth (AOD) at 550nm wavelength.

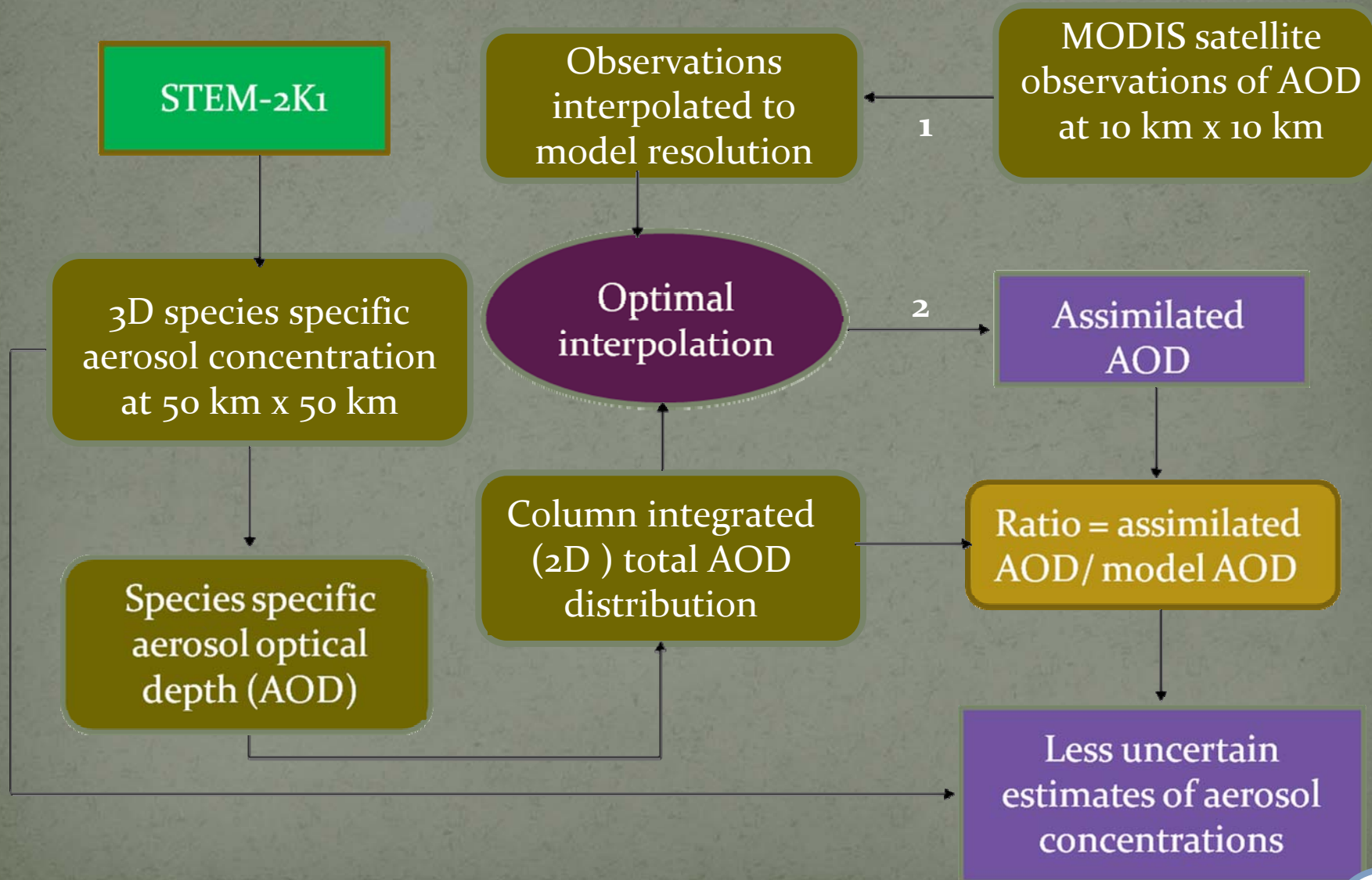
MOD04\_L2 (terra satellite) and MYD04\_L2(Aqua satellite) i.e. level 2 atmospheric aerosol product (10 km x 10 km)

- Model resolution is at 50 km  $\times$  50 km, it is more accurate to interpolate data from a finer resolution (of 10 $\times$ 10 km) onto our required model grid than to move down from yet coarser resolution of 100 $\times$ 100 km i.e. level 3.
- Level 2 AOD retrievals have quality flags ,an indicator of the quality of each parameter retrieved at the product spatial resolution

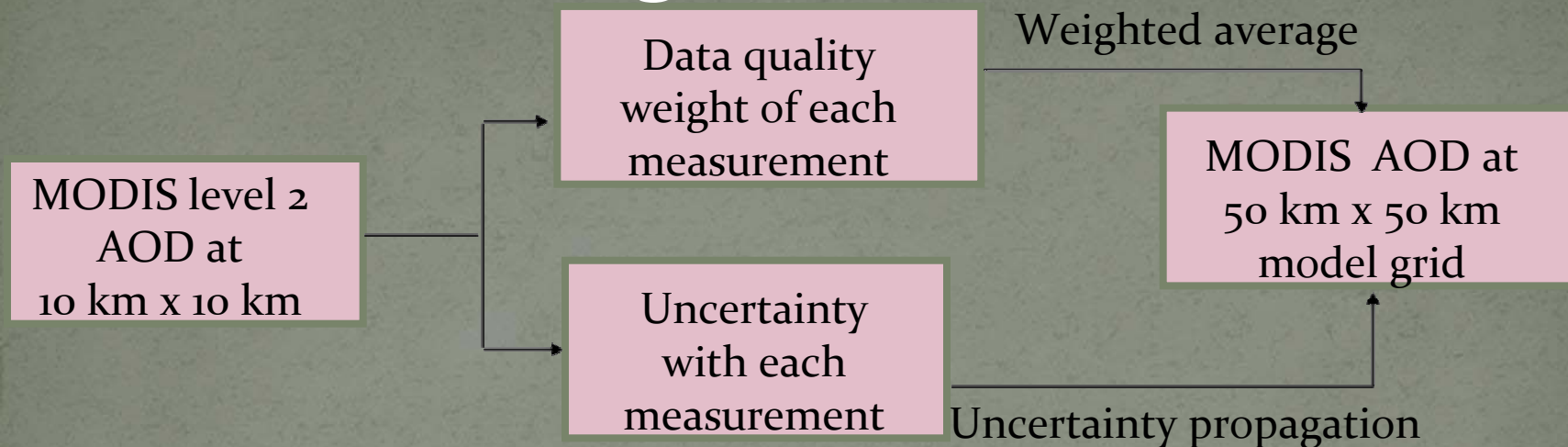
Ref: <http://modis-atmos.gsfc.nasa.gov> , <http://ladsweb.nascom.nasa.gov>



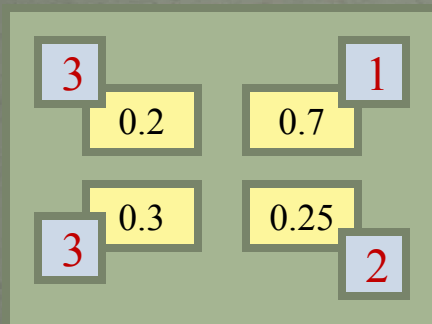
# Methodology



# Processing of satellite data



## An example calculation to explain the algorithm



Example 1 shows four valid level 2 pixels falling on a model grid of 50 km x 50 km

$$\text{Average (Av)} = 0.36 ; \text{ weighted average (Wav)} = 0.30$$

1 → Quality flags used as weights,  $w_i$

0.25 → Level 2 AOD values

Ref: MODIS Atmosphere L3 Gridded Product Algorithm Theoretical Basis Document



**Calculation of uncertainty in each level 2 measurement:** three years MODIS data (2003-2005) were validated against more reliable AERONET (AErosol RObotic NETwork) ground observations. Error associated with each level 2 AOD value was given by:

$$\Delta\text{AOD} = \pm 0.05\text{AOD} \pm 0.03 \quad \text{over ocean}$$

$$\text{and } \Delta\text{AOD} = \pm 0.15\text{AOD} \pm 0.05 \quad \text{over land [ Remer et al. (2005)]}$$

**Uncertainty propagation:** If  $\sigma_i$  be the uncertainty in each  $10 \times 10$  km valid pixel falling under a model grid where

$$\sigma_i = f_o \times \text{AOD} + e_o$$

then,

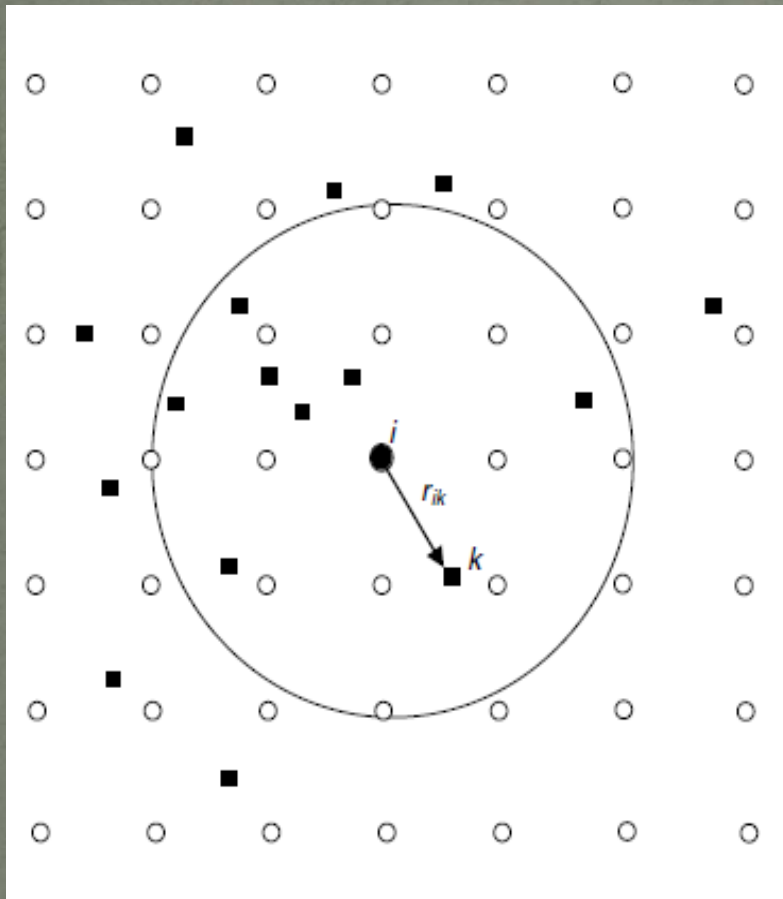
$$\text{Uncertainty}_{\text{grid}} = [\sum w_i^2 \sigma_i^2 / (\sum w_i)^2]^{1/2}$$

Continuing with example 1 illustrated before, uncertainty with the two computed averages :

$$\text{Uncertainty in Av, } \sigma_{\text{av}} = 0.054 \quad \text{and} \quad \text{Uncertainty in Wav, } \sigma_{\text{wav}} = 0.048$$



# Physical interpretation of optimal interpolation



□ grid points (circles), observations (squares), and a radius of influence around a grid point  $i$  marked with a black circle.)

1. For a target grid  $i$ , a small number of observations using empirical selection criteria are selected.
2. The background/model predicted values at these observational points, are deducted from the observational values.
3. Depending on the distances of these points from the point of interest and distances amongst themselves, weights are assigned to these points. The values now at these points are multiplied with respective weights.
4. The weighted average of these values is then added to the background value at the grid of interest to get the analysis or assimilated value at the target grid.

# Equations in Optimal interpolation algorithm

$$\tau_m' = \tau_m + K(\tau_o - H\tau_m)$$

$$K = BH^T (HBH^T + O)^{-1}$$

$$O = (f_o \tau_o + \varepsilon_o)^2 I$$

$$B_{ij} = (f_m \tau_m^i + \varepsilon_m) * (f_m \tau_m^j + \varepsilon_m) \exp \left[ -\frac{d_x^2 + d_y^2}{2l_{xy}^2} \right]$$

- ❑ **K** – Kalman gain matrix
- ❑ **H** – Interpolator from model to observation space
- ❑ **O/B** - Observed/Background error covariance
- ❑ **f** and **ε** - fractional error and RMS uncertainty
- ❑ **l<sub>xy</sub>** horizontal correlation length scale for errors in model fields
- ❑ **d<sub>x</sub>** and **d<sub>y</sub>** grid cell spacing

Adhikary et al. 2008



# Implementation of optimal interpolation algorithm

## Initial assumptions :

1. **Localization:** analysis is updated using observations within  $N_r \times N_r (=N)$  box, a subset of the huge model domain. Here,  $N_r = 5$ .
2. For the basic formulation of the code, parameter values taken were:  $f_m = 0.5$ ;  $f_o = 0.1$ ;  $e_m = 0.1$ ;  $e_o = 0.04$ ;  $l_x = l_y = l_{xy} = 5$  [Adhikary et al. (2008 )]
3. Even after localized assimilation, for greater than zero observational values, additional constraint equation.

$$\tau'_{mi} = (1-w) \tau_{mi} + w \tau_{oi}$$

$$\text{where, } 0 \leq w = B(i,i) / [O(i,i) + B(i,i)] \leq 1$$



## **New uncertainty assumptions for present study:**

1. Observational error covariance matrix was re-evaluated using uncertainty calculated while processing of satellite data

**Uncertainty propagation:** If  $\sigma_i$  be the uncertainty in each  $10 \times 10$  km valid pixel falling under a model grid where

$$\sigma_i = f_o \times \text{AOD} + e_o$$

then,  $\text{Uncertainty}_{\text{grid}} = [\sum w_i^2 \sigma_i^2 / (\sum w_i)^2]^{1/2}$

Thus , observational error covariance matrix now becomes

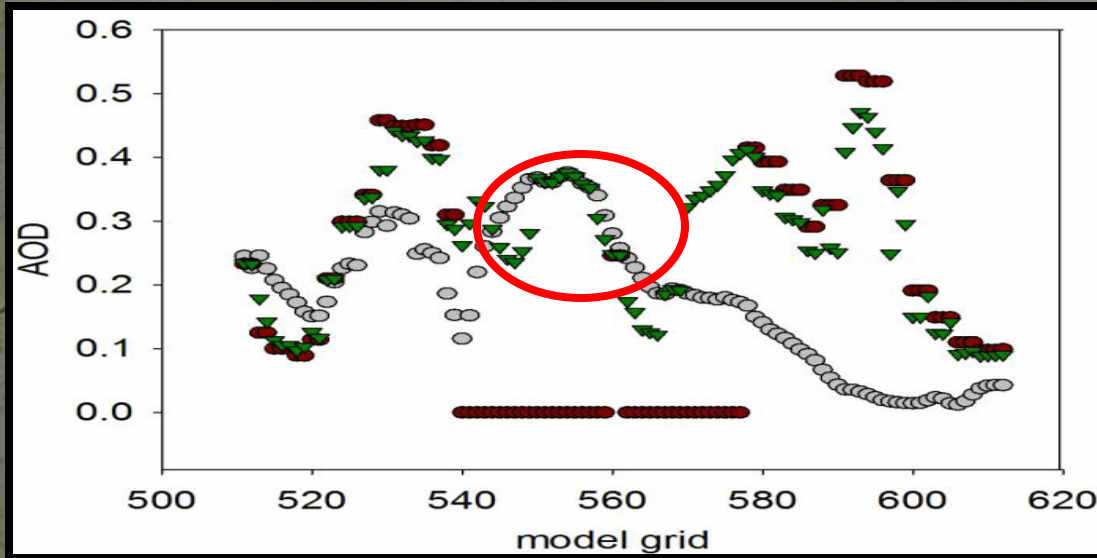
$$\mathbf{O} = (\text{Uncertainty}_{\text{grid}})^2 \mathbf{I}$$

2. Moreover, additional constraint equation is no more used for present algorithm.

# Results and discussion

## 1. Assimilation with different error covariance assumptions

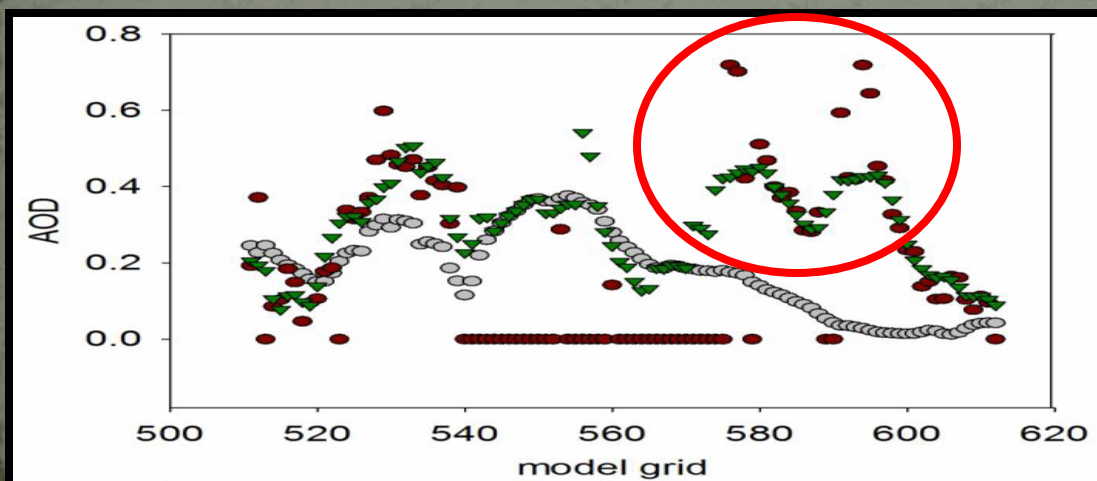
(a) Adhikary et al. (2008)



The assimilated AODs in (a) appear similar to the MODIS AODs where the latter are available.

If MODIS data were missing for a grid cell, the model predicted aerosol AODs remained more or less unchanged.

(b) Present study



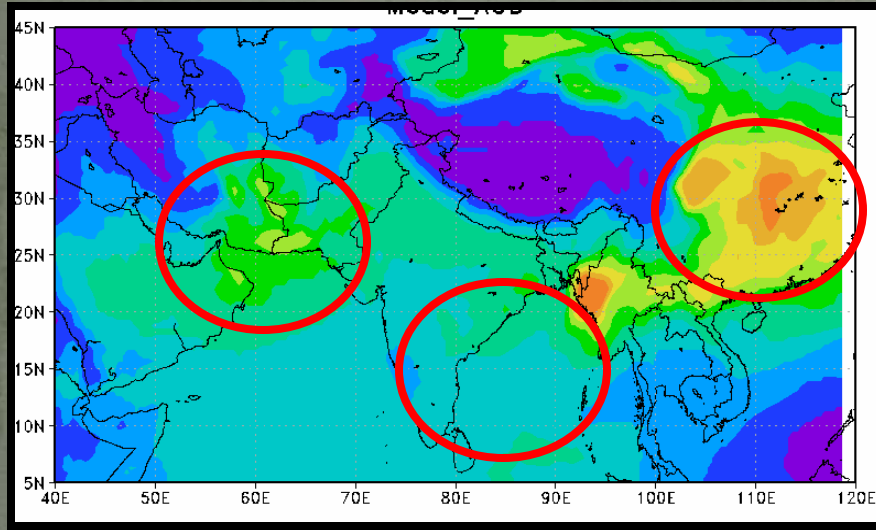
Error covariance with high AODs being high thereby assigning them less weight during the execution of the algorithm.

○ model AOD  
● MODIS AOD  
▼ assimilated AOD

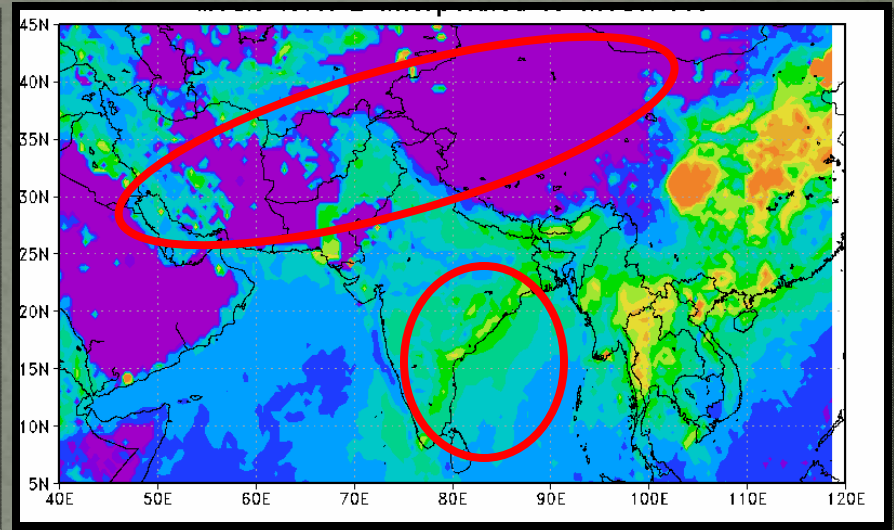


## 2. Evaluation of algorithm for March 2001

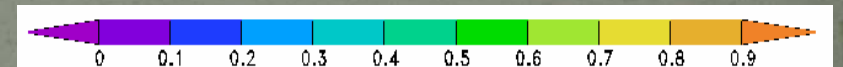
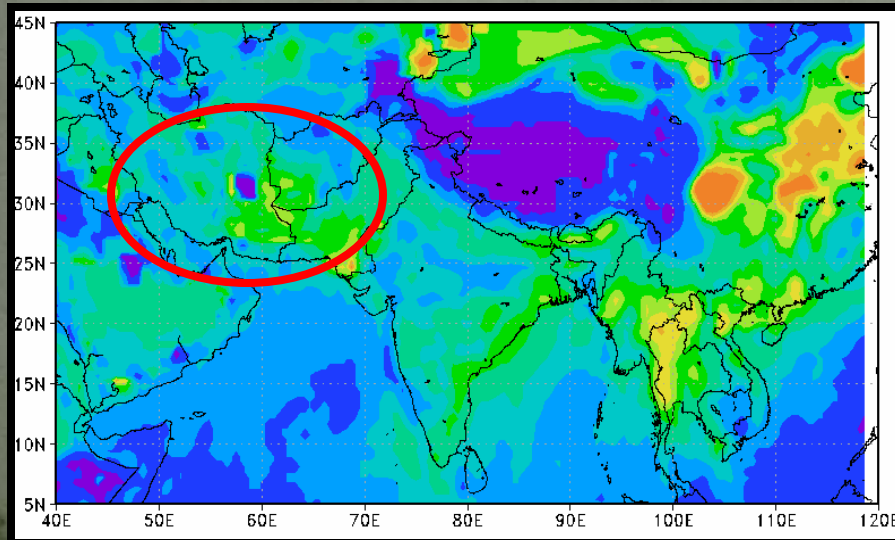
Model AOD before Assimilation



MODIS AOD



AOD after Assimilation



- ❑ Model predictions of AOD able to capture many of the major features of observed distributions. High AOD over and downwind of the major dust source regions.
- ❑ MODIS AODs more realistic but have a low spatial and temporal coverage.
- ❑ Assimilated AODs improve the model predictions



# Summary and future work

1. Data assimilation leads to more robust prediction of atmospheric variables like AOD (e.g. over Kanpur assimilated AOD was 0.37 (model predicted was xxx), very close to ground based observation  $0.35 \pm 0.023$ ).
2. Observational error covariance accounting is needed for better performance of the algorithm.
3. Other variables can be simultaneously assimilated (fine mode fraction of AOD).
4. Such offline assimilation provides a simple tool to improve CTM predictions.

*Thank You*