Satellite data assimilation of atmospheric composition



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Who am I?

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Research topics:

• Stratospheric ozone, general circulation, chemical transport modeling, with Prof. Iwasaki (Tohoku Univ.) and Dr. Shibata (MRI-JMA)

• Transport and mixing in the UTLS, with Prof. Sato and Prof. Takahashi (Univ. Tokyo) under KANTO project

• Chemical/carbon satellite data assimilation, with Dr. Eskes (KNMI), Prof. Boersma (Eindhoven Univ.) and Prof. Sudo (Nagoya Univ.)

<u>Outline</u>

- Basics on Data Assimilation
- Chemical Data Assimilation
 - Stratospheric O₃
 - Aerosols
 - Carbon cycle
 - Tropospheric chemistry
 - ? TTL studies ?

Data Assimilation Basics

Objective of Data Assimilation

is to produce a regular, physically consistent 4D representation of the state of the atmosphere from a heterogeneous array of in situ and remote instruments which sample imperfectly and irregularly in space and time.





UARS MLS ozone data at 10 hPa on 1st February 1997.

Ozone analyses at 10 hPa at 12 UTC on 1st February 1997.

Objective of Data Assimilation

is to produce a regular, physically consistent 4D representation of the state of the atmosphere from a heterogeneous array of in situ and remote instruments which sample imperfectly and irregularly in space and time.

Data assimilation

extracts the signal from noisy observations (filtering), interpolates in space and time (interpolation), and reconstructs state variables that are not sampled by the observation network (completion).

(Daley, 1997)₆

Data Assimilation Inputs

Two sources of information are used in the analysis

- observations (y)
- background (x^b) = *first guess*

In order to maintain statistical optimality, the error source statistics need to be specified,

- the observation error covariance matrix (R)
- the background error covariance matrix (B)

The Output

a maximum likelihood estimate of atmospheric state = *analysis*)

What is Data Assimilation for



- Initial state estimation for weather forecasting
- Producing reanalysis data
- Observing system design, monitoring and assessment
- Better understanding (model errors, data errors, physical process interactions, parameters, etc) (Nodet, 2012)



ECMWF atmospheric reanalysis projects

3D-OI 3D-VAR 4D-VAR 4D-VAR in ensemble context FGGE ERA-15 ERA-40 ERA-Interim ERA-CLIM

• ERA-40 (1957-2002):

Very large user base; science and downstream applications

• ERA-Interim (from 1979 onward):

Near-real time updates; better trends; better data services

• ERA-CLIM: An EU project to prepare the next generation reanalysis

Longer period; higher resolution; better input data; uncertainty information



Observations used in ERA-Interim: Instruments



Comparisons of BD circulation among reanalyses

NCEP/NCAR	1979-2001
NCEP/DOE	1979-2001
ERA-40	1979-2001
ERA-INTERIM	1989-2001
JRA-25	1979-2001

3Dvar 3Dvar 3Dvar 4Dvar

3Dvar

(Iwasaki, Hamada, Miyazaki., 2009)



ERA-40 has the strongest B-D circulation

Large contradictions are found in the tropics in JJA.

....due to many factors affecting dynamical and thermodynamical consistency

Improvements in the age-of-air calculation



(Monge-Sanz et al., 2007)

EXP471 uses an improved model with balance operator for omega-equation

To improve transport calculation, we should use 1. Forecast than analysis (Meijer et al., 2004) 2. 4D-VAR than 3D-VAR analysis (Scheele et al., 2005) 3. 3-h interval data than 6-h (Bregman et al., 2006) 4. Time-averaged data than snapshot (Pawson et al., 2007)

• 1 & 2: Dynamical consistency, balanced circulation field

• 4: Reduce transport error mainly caused by gravity waves

Best choice: 3-day forecast with 4-D VAR analysis

Chemical Data Assimilation

Stratospheric ozone Tropospheric chemistry Aerosols Carbon Cycle <u>CTM simulation</u>: large uncertainties in chemical/transport processes and boundary conditions (e.g., ozone precursor emissions)

Satellite instruments can provide strong constraints on chemical system



(NASA/Harvard univ.)

needs for advanced chemical data assimilation system to combine various obs info

Chemical Data Assimilation

- make best use of all available (satellite) data, from heterogeneous sensors, scattered in space and time
- ensure chemical and dynamical consistency
- extend analysis on non-observed species



- Weather/UV forecasting: better calculation of the radiative transfer
- Air quality/ozone hole monitoring
- Chemical reanalysis (i.e., climate simulation input)

Satellite Data Assimilation

The observation operator should contain the averaging kernel and the a priori information of each retrieval to avoid the influence of the smoothing error and the retrieval error arising from the a priori profile.

The model fields in the observation space

$$y^b = H(x) = x_a + \mathbf{A}(S(x) - x_a).$$

• The averaging kernel matrix (A) represents the sensitivity of the retrieved parameters to the true state.

• The observation operator (H) converts the model profiles to the profile that would be retrieved from satellite measurements.

$$y^{o} - y^{b} = \mathbf{A}(x_{true} - S(x)) + \epsilon,$$

The model-satellite difference (the innovation) is not biased by the a priori profile. (Rodgers, 2000; Eskes and Boersma, 2003)

Super-observation approach

- fill spatiotemporal gaps between the model and retrievals
- produce more representative data
- reduce DA computational cost







Super-obs error =

measurement error + representativeness error

- x : retrieved concentration
- y : retrieval error
- w : weight (coverage area for most cases)
- m :number observation in a super-obs pixel
- c : correlation among data

A Japanese chemical data assimilation project (2009-2012)

- We (MRI-JMA, NIES, JAMSTEC, Tohoku Univ.) have developed chemical data assimilation systems for monitoring atmospheric environment in East Asia and over the globe.
- The data assimilation systems developed by the four research institutes employed a same assimilation scheme (<u>EnKF</u>).

→ Impact of the model performance on data assimilation

• The approach allows to simultaneously optimize forecast variables (i.e., concentrations) and parameters (i.e., emissions).



Ensemble Kalman Filter

	4D-Var	4D-EnKF
Background error statistics	Flow-dependent	Flow-dependent
Program code	Complicated	Simple
Adjoint matrix	Necessary	Unnecessary
Observation operator	Requires tangent linear & adjoint operators	Requires only a forward transform operator
Asynchronous observations	Handles at each observational time	Handles at each observational time
Analysis error covariance	Not provided	Explicitly provided

(Kalnay et al., 2007)

EnKF data assimilation: An ensemble

Kalman filter (EnKF) is an advanced data assimilation technique in which the **forecast error covariance is advanced by the model itself** (i.e., flow-dependent forecast error covariance). The advanced approach allow us to **fully take advantage of CTMs**.



Background error covariance

$$\overline{\mathbf{x}^{b}} = \frac{1}{k} \sum_{i=1}^{k} \mathbf{x}_{i}^{b}; \ \mathbf{X}_{i}^{b} = \mathbf{x}_{i}^{b} - \overline{\mathbf{x}^{b}}.$$
$$\mathbf{P}^{b} = \mathbf{X}^{b} (\mathbf{X}^{b})^{T}.$$

Observation operator

$$\mathbf{y}_{i}^{b} = H\left(\mathbf{x}_{i}^{b}\right)$$
$$\mathbf{y}_{i}^{b} = H\left(\mathbf{x}_{i}^{b}\right) = \sum_{i=1}^{k} a_{i} \mathbf{x}_{i}^{b},$$

Analysis error covariance

$$\begin{split} \tilde{\mathbf{P}}^{a} &= \left[\frac{\left(k-1\right)\mathbf{I}}{1+\Delta} + \left(\mathbf{Y}^{\mathbf{b}}\right)^{T} \mathbf{R}^{-1} \mathbf{Y}^{\mathbf{b}} \right]^{-1}, \\ \mathbf{T} &= \left[\left(k-1\right) \tilde{\mathbf{P}}^{a} \right]^{1/2} \end{split}$$

Analysis (incl. perturb.)update

$$\overline{\mathbf{x}}^{a} = \overline{\mathbf{x}}^{b} + \mathbf{X}^{b} \widetilde{\mathbf{P}}^{a} \left(\mathbf{Y}^{b}\right)^{T} \mathbf{R}^{-1} \left(\mathbf{y}^{o} - \overline{\mathbf{y}^{b}}\right)$$
$$\mathbf{X}^{a} = \mathbf{X}^{b} \mathbf{T}$$

Simultaneous optimization of state and parameter in EnKF

Background error covariance (Xb)



The state vector augmentation technique allows us to simultaneously estimate the model state (i.e., concentration) and the uncertain model parameter (i.e., emission).



(Miyazaki et al., 2012a)

Emission estimation: A state vector which includes both the concentrations and the emissions makes it possible to find the optimal values for the emissions.

C2H4

N2O5

NOx

Ox

HACT COST CONTROL



0.75

0.6

0.45

0.3

0.15

-0.15

-0.3

-0.45

-0.6

-0.75

Š Š

0

Background error covariance structure in EnKF Surface 500 hPa CO-sflux CO-sflux NOx-sflux NOx-sflux LNOx LNOx **SO4** 504 DMS DMS SO2 SO2 OXS OXS MACROOH MACROOH CH3COOOH HOROOH CH3COOOH HOROOH ISOOH ISOOH C3H7OOH C3H7OOH C2H5OOH C2H5OOH СНЗООН CH3OOH ISON ISON **MPAN MPAN** PAN PAN MACR MACR HACET HACET MGLY MGLY NALD NALD **СН3СНО CH3CHO** CH2O CH2O CH3COCH3 CH3COCH3 C10H16 C10H16 C5H8 C5H8 ONMV ONMV C3H6 C3H6 C2H4 C3H8 C3H8 C2H6 C2H6 CO CO H2O2 H2O2 HNO4 HNO4 HNO3 HNO3

N2O5

NOX

-sfl 's ŠÖ Ox

4648602433055 4648602433

(Miyazaki et al., 2012b)

1. Stratospheric ozone (MLS, OMI)

2. Aerosols

(CALIPSO, ground-based lidar)

Japanese CTMs/CCMs & 3D/4D-LETKF

> ?TTL water vapor? still very challenging!

3. Surface CO2 flux (GOSAT, CONTRAIL) 4. Air quality (OMI, SCIAMACHY...)

1. Stratospheric ozone

Forecast models:

(1) CCSR/NIES CCM (Akiyoshi et al., 2009)

T42L34 p-top=0.01 hPa

(2) MRI CCM2 (Shibata and Deushi, 2008, Deushi and Shibata 2011)

T42L68 p-top=0.01 hPa

(3) **CHASER** (Sudo et al., 2002) *not shown here*

T42L32 p-top=3 hPa

The multi-model comparison provides an opportunity to examine the effects of the model bias on the assimilation performance.

Assimilated data: MLS O3 profile, OMI O3 column, JCDAS (met. data) Control variables: O3, U, V, T Assimilation setting: 3D analysis with 6-hourly cycle

Ozone data assimilation

Improvements by MLS O3: throughout the stratosphere. Improvements by OMI-TO3: only in the lower stratosphere.

(Nakamura, Miyazaki, et al., submitted)





- NIES: O₃ assimilation → SW heating 10 % → net radiative heating 40% (→ might also influence chemical reaction (under investigation)) chemistry-climate coupling data assimilation is important !
- MRI: dynamics or radiation calculation problem?



2. Aerosols

under development by JMA (T. Sekiyama)

- Asian Dust
 - seasonal phenomenon sporadically affecting East
 Asian countries during the springtime,
 - causes health and aviation problems,
 - originates in the deserts of Mongolia and China.

Forecast models: MASINGAR

Assimilated data: Satellite (CALIPSO/CALIOP) and ground-based lidar

Control variables: dust (partitioned into 10-size bins), dust flux, sea-salt, OC, BC, and sulfate aerosols

Assimilation setting: 4D analysis with 48-h time window

Operational dust prediction



- JMA wants to utilize aerosol data assimilation for improving their operational dust prediction.
- If possible, they want to use the aerosol analysis for their NWP and climate simulations.

- The Model of Aerosol Species in the Global Atmosphere (MASINGAR) of MRI/JMA simulates...
- dust (partitioned into 10-size bins), sea-salt, OC, BC, and sulfate aerosols







Satellite Lidar observation (CALIPSO/CALIOP): NASA launched the polarorbit satellite in 2006.

Ground-based lidar network (NIES AD-Net): NIES Japan is operating more than 20 lidar stations in East Asia.







Contours and gray shades are **surface dust concentrations**.

(a) Free model-run result without data assimilation.
(b) CALIPSO data assimilation result.

Red and blue circles are weather stations.

Red ones observed aeolian dust.

Blue ones did not observe any dust events.

The shape of the high AOD detected by MODIS are consistent with the surface dust analysis.

Dust emission inverse analysis by EnKF



The dust concentrations in the downwind region are evidently improved when this dust emission analysis is installed to the model simulation.

JMA's plan for aerosol prediction

 The EnKF aerosol analyses as initial conditions of aerosol prediction.

(hopefully, in practical use by 2014...)

• Aerosol reanalysis:

available for climate modeling?

- Aerosol climatology (detailed): available for NWP?
- Ideally, weather-chemistry coupled DA...



3. Surface CO₂ flux

- establish a 4D-EnKF data assimilation system to estimate global surface CO₂ fluxes from various data.
- evaluate the potential impacts of various data obtained from the surface network, satellite (GOSAT), and aircraft (CONTRAIL) measurements, using observational system simulation experiments (OSSEs).

Forecast models: MJ98-CDTM, FRCGC ACTM Assimilated data: Satellite (GOSAT), Aircraft (CONTRAIL), Ground-based network Control variables: Surface CO₂ flux, Atmospheric CO₂ concentration Assimilation setting: 4D analysis with 7-day time window (Miyazaki, 2009, Miyazaki et al., 2011)



Observation System Simulation Experiments (OSSEs)

- demonstrate the performance of the DA scheme with known errors
- tell us how much error reductions
 can be expected by each dataset

(Miyazaki et al., 2011)

Flux error reduction rate [%]: grid-scale

(a) Surface network

(b) GOSAT







(Miyazaki et al., 2011)

Flux error reduction rate [%]: regional-fluxes



CONTRAIL data: Europe and Asia. (Miyazak GOSAT data: North and South America, South Africa, Asia, and Europe

Flux error reduction rate [%]: regional-fluxes



Additional constraints are required especially over North Africa, tropical South America, southern North America, and the oceans. (Miyazaki et al., 2011)

4. Air quality (tropospheric chemistry)

<u>Forecast models</u>:

(1) **CHASER** (Sudo et al., 2002)

T42L32 p-top=3 hPa

(2) MRI CCM (Shibata and Deushi, 2008) T42L68 p-top=0.01 hPa

 for monitoring Asian/global atmospheric environment

Assimilated data: OMI NO2, SCIAMACHY NO2, TES O3, etc...

Control variables: NOx emission, NO2, O3, HNO3, etc...

Assimilation settings: 3D-analysis

(Miyazaki et al., 2012a, 2012b)

Tropospheric chemical data assimilation

- ✓ The use of data assimilation for atmospheric chemistry (e.g., MACC, NASA/DAO, JPL, BASCOE), especially for short-lived chemical species, is still challenging.
- ✓ The tropospheric chemical system is stiff. Small perturbations are damped out quickly in time. A large part of the chemical system is not sensitive to initial conditions, but is sensitive to the model parameters (e.g., emissions). → Simultaneous adjustment of model parameters (e.g., emissions) and concentrations is a powerful framework.
- ✓ The advantage of Ensemble Kalman filter (EnKF) is its easy implementation for complicated systems; i.e., without development of adjoint code for CTMs.



-45 45

TES O3 & CO





TES, MLS, OMI on AURA MOPITT on TERRA



(KNMI)

Averaging kernel

0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4

Tropospheric NO2 observations from space :

GOME	1995-2003	40 x 320 km	10:30 AM LT
SCIAMACHY	2003-	60 x 30 km	10:00 AM LT
OMI	2004-	13 X 24 km	1:30 PM LT
GOME-2	2007-	40 X 80 km	9:30 AM LT



MOPITT on TERRA











Absorbing Aerosols (BC)

MOPPIT CO

(based on a MIT lecture note)

Aerosols

OMI NO₂

CHASER-DAS (Miyazaki et al., 2012a, 2012b)

Assimilation scheme	Local ensemble transform Kalman filter (Hunt et. al., 2007)
Forecast model	CHASER (Sudo et al., 2002)
A priori emissions	EDGAR3.2 + GFED2 + REAS1 + GEIA, Price and Rind (1992)
State vector	NOx & CO emissions, lightning NOx, 35 chemical species
Obs operator	Averaging kernel and a priori information
Super Obs	applied for OMI NO ₂ and MOPPIT CO data
Cycle	100 min.
Techniques	Spatial/variable covariance localization, covariance inflation
Assimilated data	OMI NO ₂ (DOMINO2), TES O ₃ (ver. 4), MOPITT CO (ver. 5), MLS O ₃ & HNO ₃ (ver. 3.3)
Validation data	SCIAMACHY NO ₂ , GOME-2 NO ₂ , TES CO, Ozonesonde (WOUDC/ SHADOZ), Aircraft (INTEX-B)



<u>Self-consistency check</u>: Observation-minus-Forecast (OmF)



<u>Self-consistency check</u>: Chi-square test

An important test for the quality of data assimilation is whether the differences between the innovations are consistent with the covariance matrices for the model forecast and observations.

$$\mathbf{Y} = \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

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$$= \frac{1}{\sqrt{m}} (\mathbf{H}\mathbf{P}^{b}\mathbf{H}^{T} + \mathbf{R})^{-1/2} (\mathbf{y}^{o} - H(\mathbf{x}^{b})). \qquad \chi^{2} = \operatorname{trace} \mathbf{Y}\mathbf{Y}^{T}$$

Google



v.s. Ozone sonde (JUL)



SH



v.s. INTEX-B aircraft data



Validation

Spatial correlation diff. (=assim-model) BIAS reduction rate (=(model-assim)/model*100) RMSE reduction rate (=(model-assim)/model*100)





















for the future development of both models and observations

Analysis spread

requirement for further constraints from additional observations or high quality data

O3 700 hPa



Analysis increment

useful to identify sources of the model error and improve the performance



Summary

Data assimilation is a powerful tool to make best use of all available observation data and study chemical/physical processes.

Advanced chemical data assimilation systems have been developed to combine observations of chemical compounds from multiple satellite.

The assimilation of individual data sets results in a strong influence on both assimilated and non-assimilated species through the interspecies error correlation and the chemical coupling.

The simultaneous adjustment of the emissions and concentrations is a powerful approach to correcting the tropospheric ozone budget and profile analyses.

Data assimilation for TTL studies

- Chemistry-climate coupling data assimilation (incl. H₂O) framework might be useful for better understanding chemistry/radiation/dynamics interactions controlling the TTL structure/variability (but might be strongly model-dependent).
- Aircraft data is expected to provide important constraints on the chemical states and the radiative forcing in the TTL region (but perhaps available only on campaign basis).
- still need to increase observations (number, resolution, e.g., GPS) and improve models (e.g., convective and microphysics parameterizations, resolution, diurnal variations).
- General circulation: Direct wind observations and momentum/heat budget information from any observations would be helpful.
- Very challenging

- <u>Miyazaki et al.</u>, Simultaneous assimilation of satellite NO2, O3, CO, and HNO3 data for the analysis of tropospheric chemical composition and emissions, ACP, 2012. (Chemical simultaneous DA)
- <u>Miyazaki et al.</u>, Global NOx emission estimates derived from an assimilation of OMI tropospheric NO2 columns,, ACP, 2012. (OMI NO2 DA)
- <u>Miyazaki et al.</u>, Assessing the impact of satellite, aircraft, and surface observations on CO₂ flux estimation using an ensemble-based 4D data assimilation system, JGR, 2011. (CO₂ DA system, OSSE study)
- <u>Miyazaki</u>, Performance of a local ensemble transform Kalman filter for the analysis of atmospheric circulation and distribution of long-live tracers under idealized conditions, JGR, 2009. (CO₂ DA system, OSSE study)
- <u>Miyazaki et al.</u>, Formation mechanisms of latitudinal CO₂ gradient in the upper troposphere over the subtropics and tropics, JGR., 2009 (CO₂ transport/aircraft data analysis)
- <u>Miyazaki et al.</u>, Global-scale transport of carbon dioxide in the troposphere, JGR, 2008. (CO₂ transport/modeling)
- <u>Maki et al.</u>, New techniques to analyze global distributions of CO₂ concentrations and fluxes from non-processed observational data, Tellus, 2010. (QC for DA)
- <u>Maki et al.</u>, The Impact of Ground-Based Observations on the Inverse Technique of Aeolian Dust Aerosol, SOLA, 2011. (Dust emission inversion)
- Sekiyama et al., Data assimilation of CALIPSO aerosol observations. ACP, 2010. (Aerosols DA)
- <u>Sekiyama et al.</u>, The Effects of Snow Cover and Soil Moisture on Asian Dust: II. Emission Estimation by Lidar Data Assimilation, SOLA, 2011. (Aerosols DA)
- <u>Sekiyama et al.</u>: A simulation study of the ensemble-based data assimilation of satellite-borne lidar aerosol observations, GMDD., 2012. (Aerosols OSSE)
- <u>Iwasaki et al.</u>, Comparisons of Brewer-Dobson Circulations diagnosed from Reanalyses, JSMJ, 2009. (BD inter-comparison among reanalyses)