Atmospheric Composition Data Assimilation: Selected topics

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Atmospheric composition: A strongly constrained system

- Coupling with the meteorology is in each 3D grid volume (winds, temperature, humidity, clouds/radiation)
- Chemical solution is also controlled by chemical sources and sinks

Boundary layer $O_3$
Forecast verification after $O_3$ assimilation

no $O_3$ assimilation
with $O_3$ assimilation
Atmospheric composition as a slaved /controlled system

- As coupled system have to consider the Information content:
  - Chemical model
  - Chemical observations
  - Meteorology

- Favors online chemistry-meteorology models

- No for Incremental formulation with a lower resolution chemistry

- Because the control of meteorology on chemistry is so strong, the feedback of chemistry on meteorology is small

- Except for long-lived species, chemical forecast is not the most useful product, but analyses are

- Forecast improvement is better addressed with parameter (e.g. sources) estimation
### Notation and definitions

Continuity equation; $\rho$  dry air density

\[
\frac{1}{\rho} \frac{D\rho}{Dt} + \nabla \cdot \mathbf{V} = 0 \quad \text{Lagrangian} \quad ; \quad \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \quad \text{Eulerian}
\]

Mixing ratio $c_i$ of constituent $i$ is defined as $c_i = \frac{\rho_i}{\rho}$

\[
\frac{Dc_i}{Dt} = 0 \quad \text{Lagrangian} \quad ; \quad \frac{\partial c_i}{\partial t} + \mathbf{V} \cdot \nabla c_i = 0 \quad \text{Eulerian}
\]

The consistency between the wind field $\mathbf{V}$ used for the continuity equation and the wind field $\mathbf{V}$ used for the transport of the constituent $i$ is called the **mass consistency**

**CTM** (Chemical Transport Models) are **offline** (from meteorology) models that uses different $\mathbf{V}$ and often at different resolution: they were introduced to use met analyses

**Online** chemical models have mass consistency and same resolution as the meteorology
GEM-BACH online with meteo model / BASCOE CTM offline model driven by 6-hourly meteorological analyses

Validation with MIPAS OFL
20030825-20030904, 60°N-90°N

- GEM-BACH, EC 4D-VAR (K4BCS304)
- GEM-BACH, EC 3D-VAR (K3BCS304)
- BASCOE CTM, EC 3D-VAR (v3s85)
- BASCOE CTM, ECMWF (d2003G)
Coupled Assimilation $O_3$/meteorology

Assimilation of limb sounding MIPAS observations of $O_3$ with AMSU-A

MIPAS vertical resolution 1-3 km

- solid lines
- no radiation feedback
- dashed lines
- assim $O_3$ used in radiative scheme (k-correlated method)

de Grandpré et al., 1997, MWR
Operational air quality analysis

Analysis of $O_3$, NO$_2$, SO$_2$, PM$_{2.5}$, PM$_{10}$ each hour

*experimental since 2002, operational since Feb 2013*

**History**

- $O_3$, PM$_{2.5}$ – using CHRONOS 2002-2009
- $O_3$, PM$_{2.5}$ – using GEM-MACH 2009-2015
- $O_3$, PM$_{2.5}$, NO$_2$, SO$_2$, PM$_{10}$ since April 2015 (Robichaud et al. 2015, *Air Qual Atmos Health*)
- Multi-year data set (2002-2012) (Robichaud and Ménard 2014, ACP)
What does the medicine has to say about air pollution?

- Interact with many groups (e.g. Health Canada, Environmental Cardiology)

  - In terms of mass, we breathe-in per day about 20 kg of air, 2 kg of liquid and 1 kg of solid food

    12-25 breath per minutes each is about 1 liter
    \(\approx 20,000\) liter of air/day

- Pulmonology and cardiology are strongly linked
Filtered air

Polluted air  Mean 15 μg/m³

Normal Chow

Sun et al., JAMA 2005

High-Fat Chow
Canadian Census Health and Environmental Cohort (CanCHEC) and the Canadian Urban Environmental Health Research Consortium (CANUE)

www.canue.ca

Brook et al. BMC Public Health (2018) 18:114
Evaluation of analysis by cross-validation (or leave-out observations)


Ménard, R and M. Deshaies-Jacques Part II: Diagnostic and optimization of analysis error covariance. *Atmosphere* 2018, 9(2), 70; doi: [10.3390/atmos9020070](https://doi.org/10.3390/atmos9020070)
3 spatially random distributed set of observations
\text{var}(O-A) [O3]

Passive /independent obs.
\text{var}(O_1 - A(O_2, O_3))
\text{var}(O_2 - A(O_1, O_3))
\text{var}(O_3 - A(O_1, O_2))

Active obs.
\text{var}(O_1 - A(O_1))
\text{var}(O_2 - A(O_2))
\text{var}(O_3 - A(O_3))
Estimation of error covariances in observation space \((HBH^T, R)\)

**Theorem on estimation of error covariances in observation space**

Assuming that observation and background errors are uncorrelated, the necessary and sufficient conditions for error covariance estimates to be equal to the true observation and background error covariances are:

1) \( \mathbb{E}[(O-B)(O-B)^T] = HBH^T + \tilde{R} \)  \( \text{Innovation covariance consistency} \)

A scalar version of this condition is

\[
tr\left\{ \mathbb{E}[dd^T] (HBH^T + \tilde{R})^{-1} \right\} = \mathbb{E}\left\{ tr[ d^T (HBH + \tilde{R})^{-1} d ] \right\} = \mathbb{E}[\chi^2] = N_p
\]

or

\( J_{\text{min}} = N_p / 2 \)

2) \( HK = H\tilde{K} \)  \( \text{The Kalman gain condition} \)

Ménard, 2016, QJRMS
Diagnostic of the Kalman gain condition

- Daley 1992 (MWR) suggested that the time lag-innovation covariance to be equal zero (assuming observation errors are serially uncorrelated)
- Here we suggest to use cross-validation

Simple interpretation with a scalar problem

1) Innovation consistency says that the **sum** of observation and background error variances is the sum of the true error variances

2) Kalman gain condition says that the **ratio** of observation to background error variance is the ratio of the true error variances
Hilbert spaces of random variables

Define an inner product of two (zero-mean) random variables $X$, $Y$ as

$$\langle X, Y \rangle = \mathbb{E}[XY]$$

Can defined a metric as

$$\|X\|_2 = \sqrt{\mathbb{E}[X^2]}$$

Uncorrelated random variables $X$, $Y$ would be orthogonal $\langle X, Y \rangle = 0$
Verification of analysis by cross-validation:
A geometric view

obs and background errors are uncorrelated
\[ E[\mathbf{\varepsilon}^o (\mathbf{H} \mathbf{\varepsilon}^f)^T] = 0 \quad \Rightarrow \quad E[(O - B)(O - B)^T] = \mathbf{R} + \mathbf{H B H}^T \]

active and independent obs. errors are uncorrelated
\[ E[\mathbf{\varepsilon}^o (\mathbf{\varepsilon}_c^o)^T] = 0 \]
\[ E[\mathbf{H} \mathbf{\varepsilon}^f (\mathbf{\varepsilon}_c^o)^T] = 0 \]
\[ E[(\mathbf{H}_c \mathbf{\varepsilon}^a) (\mathbf{\varepsilon}_c^o)^T] = 0 \]
Verification of analysis by cross-validation: A geometric view

\[
E[(H_c \epsilon^a)(\epsilon_c^o)^T] = 0 \quad \Rightarrow \quad E[(O - A)(O - A)^T_c] = R_c + H_c A H_c^T
\]
Verification of analysis by cross-validation: A geometric view

by varying the observation weight while we can find a true optimal analysis

\[ E[(O - B)(O - B)^T] = R + HBH^T \]
Verification of analysis by cross-validation: A geometric view

Hollingsworth-Lönnberg 1989

\[ \mathbb{E}[(O - \hat{A})(O - \hat{A})^T] = R - \mathbf{H} \hat{\mathbf{A}}_{HL} \mathbf{H}^T \]
Verification of analysis by cross-validation: A geometric view

\[ E[(\hat{A} - B)(\hat{A} - B)^T] = HBH^T - \hat{H}A_{MDJ}H^T \]
Verification of analysis by cross-validation: A geometric view

Desroziers et al. 2005

\[ E[(O - \hat{A})(\hat{A} - B)^T] = H\hat{A}_D H^T \]

Geometrical proof given in Ménard and Deshaies-Jacques 2018
Verification of analysis by cross-validation: A geometric view

Diagnostic in passive observation space we get

\[ E[(\hat{A} - B)_c (\hat{A} - B)_c^T] = H_c B H_c^T - H_c \hat{A}_{MDJ} H_c^T \]

The yellow triangle we have

Analysis plane

\[ \begin{align*}
E[(O - B)_c (O - B)_c^T] &= E[(\hat{A} - B)_c (\hat{A} - B)_c^T] \\
&+ E[(O - \hat{A})_c (O - \hat{A})_c^T] 
\end{align*} \]

and using

\[ \begin{align*}
E[(O - \hat{A})_c (O - \hat{A})_c^T] &= H_c \hat{A} H_c^T + R_c \\
E[(O - B)_c (O - B)_c^T] &= H_c B H_c^T + R_c 
\end{align*} \]
Application to $O_3$ surface analysis

Iter 0 (first guess error correlation)
Iter 1 (Maximum Likelihood estimation of correlation length)

Input error statistics

<table>
<thead>
<tr>
<th>Experiment</th>
<th>$L_c$ (km)</th>
<th>$\langle (O-B)^2 \rangle$</th>
<th>$\hat{\gamma} = \hat{\sigma}_o^2 / \hat{\sigma}_b^2$</th>
<th>$\hat{\sigma}_o^2$</th>
<th>$\hat{\sigma}_b^2$</th>
<th>$\chi^2 / N_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_3$ iter 0</td>
<td>124</td>
<td>101.25</td>
<td>0.22</td>
<td>18.3</td>
<td>83</td>
<td>2.23</td>
</tr>
<tr>
<td>$O_3$ iter 1</td>
<td>45</td>
<td>101.25</td>
<td>0.25</td>
<td>20.2</td>
<td>81</td>
<td>1.36</td>
</tr>
</tbody>
</table>

Estimate of analysis error variance at passive observation sites

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Passive $\text{diag}(H_c \hat{A}_{MDJ} H_c^T)$</th>
<th>Passive $\text{var}[(O - \hat{A})<em>c] - \sigma</em>{oc}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_3$ iter 0</td>
<td>26.03</td>
<td>32.72</td>
</tr>
<tr>
<td>$O_3$ iter 1</td>
<td>28.95</td>
<td>28.75</td>
</tr>
</tbody>
</table>

Estimation of active analysis error variance

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Active $\text{diag}(H_{\hat{A}_{MDJ}} H^T)$</th>
<th>Active $\text{diag}(H_{\hat{A}_{DL}} H^T)$</th>
<th>Active $\text{diag}(H_{\hat{A}_{HL}} H^T)$</th>
<th>Active $\text{diag}(H_{\hat{A}_{P}} H^T)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_3$ iter 0</td>
<td>22.69</td>
<td>9.61</td>
<td>-6.03</td>
<td>5.77</td>
</tr>
<tr>
<td>$O_3$ iter 1</td>
<td>13.32</td>
<td>13.68</td>
<td>8.94</td>
<td>11.60</td>
</tr>
</tbody>
</table>
Verification of analysis by cross-validation: when active observation and background errors are correlated

\[ X = E[\varepsilon^f (\varepsilon^o)^T] \]

\[ Hx^a - Hx^f = H(BH^T - X)(HBH^T + R - X^T H^T - HX)^{-1} \]
Verification of analysis by cross-validation:
when active observation and background errors are correlated

\[ X = \rho \sigma_b \sigma_o \]

\[ (A - B) = (\sigma_b^2 - \rho \sigma_b \sigma_o) \left( \sigma_b^2 + \sigma_o^2 - 2\rho \sigma_b \sigma_o \right)^{-1} \]

The HL and MDJ diagnostic continue to be valid but not the D diagnostic
Verification of analysis by cross-validation:
when active observation and background errors are correlated

when $X = 0$
$(A - B) < (O - B)$
when $\rho > \sigma_o / \sigma_b$
$(A - B) > (O - B)$
Simple model: **Random proportional tendencies**

\[
\frac{c_i - c_{i-1}}{\Delta t} = \varepsilon_i c_{i-1}
\]

where \(\varepsilon\) is random parameter. Suppose we divide a time interval \([0,1]\) into \(K\) \(\Delta t\) intervals

\[
\sum_{i=1}^{K} \left( \frac{c_i - c_{i-1}}{c_{i-1}} \right) = \Delta t \sum_{i=1}^{K} \varepsilon_i
\]

we can approximate

\[
\sum_{i=1}^{K} \left( \frac{c_i - c_{i-1}}{c_{i-1}} \right) \approx \frac{c(t_K)}{c(t_0)} dc = \log c(t_K) - \log c(t_0)
\]

and by central limit theorem

\[
\Delta t \sum_{i=1}^{K} \varepsilon_i = \Delta t K \left( \frac{1}{K} \sum_{i=1}^{K} \varepsilon_i \right) \sim N(\mu, \sigma^2)
\]
\[ \log \frac{c(t_K)}{c(t_0)} \sim N(\mu, \sigma^2) \]

then

\[ \frac{c(t_K)}{c(t_0)} \sim LN(\mu, \sigma^2) \]

is lognormally-distributed.
Analysis step

Positive analysis (lognormal formulation) (Cohn 1997, Fletcher and Zupanski 2006)

Letting $w = \log c$, the analysis equation is then of the form

$$w^a = w^f + \overline{K}(w^o - Hw^f - b)$$

$$\overline{K} = \overline{B}^f H^T \left( H\overline{B}^f H^T + \overline{B}^o \right)^{-1}$$

where the $\overline{B}$ s are the error covariances defined in log space.

$b$ is an observational correction, and has different form whether we consider that:

a) the measurement in log space that is unbiased (in which case $b = 0$)
b) the measurement in physical space is unbiased $b_i = -\overline{B}_{ii}/2$

Transformation of mean and covariance between log and physical quantities

$$\langle c_i \rangle = \exp \left[ \langle w_i \rangle + \frac{1}{2} \overline{B}_{ii} \right]$$

$$P_{ij} = \langle c_i \rangle \langle c_j \rangle [\exp(\overline{B}_{ij}) - 1]$$
Inverse transformation $\bar{B}_{ij} = \log \left( 1 + \frac{P_{ij}}{\langle c_i \rangle \langle c_j \rangle} \right)$ and with $P_{ij} = \sigma_i^f \sigma_j^f C_{ij}^f$

and a relative standard deviation $\delta = \frac{\sigma}{\langle c \rangle}$ then

$$\bar{B}_{ij} = \log \left( 1 + \delta_i^f \delta_j^f C_{ij}^f \right) \approx \delta_i^f \delta_j^f C_{ij}^f \quad \text{for} \quad \delta \leq 0.1$$
Data assimilation with a relative error formulation

If the state-dependent observation error is dependent on the forecast instead of the truth, i.e.

\[ \mu_k^o = H_k \mu_k^t + g_k(H_k \mu_k^f) \circ \epsilon_k. \]

and that the state-dependent model error is dependent on the analysis instead of the truth

\[ \mu_{k+1}^f = M_k \mu_k^a + f_k(\mu_k^a) \circ \epsilon_k^q, \]

Then the Bayesian update, and KF propagation using the proper conditional expectation can be derived and give the standard KF with

\[ R_k \circ [g_k(H_k \mu_k^f)g_k^T(H_k \mu_k^f)] = R_k^o. \]
\[ Q_k = f_k(\mu_k^a)f_k^T(\mu_k^a) \circ C_k^q. \]

Ménard et al., 2000. MWR
4.4 Lognormal KF

- KF relative error formulation
  \[ \varepsilon^o = \mu^f \circ \tilde{\varepsilon}^o \]
  \[ \varepsilon^q = \mu^a \circ \tilde{\varepsilon}^q \]

- KF lognormal formulation
Lognormal distributions: \[ \sigma_c^2 = \langle c \rangle^2 \exp(\sigma_w^2 - 1) \]

Observation errors is not lognormally distributed

Observations at low concentrations can have negative values, because there are detection limits, or because of the retrieval observations

\[ \sigma_c = \langle c \rangle \cdot cte + b \]

model values at observation sites

\[ \sigma_c = \langle c \rangle \cdot cte \]
Lognormal or something else?

Process of random dilution

$n$ is the number density (number of molecules per unit volume), $v$ is the volume, and $q$ is total number of molecules

$$q = n v$$

If all these molecules found themselves into a larger volume $V$, then the new number density is

$$q = N V$$

thus

$$N = n \left( \frac{v^\alpha}{V} \right) = n \alpha$$

where $\alpha$ is a dilution factor

$0 < \alpha < 1$

And after $k$ dilutions,

$$n_k = n_0 \prod_{i=1}^{k} \alpha_i \quad \text{or} \quad \ln n_k = \ln n_0 + \sum_{i=1}^{k} \ln \alpha_i$$

If $\alpha_i \sim U(0,1)$ then $-\log \alpha_i \sim EXP(1)$ and $-\sum_{i=1}^{K} \log \alpha_i \sim Gamma(k,1)$

so $n_k \sim Log-Gamma$ distribution
Thanks