Atmospheric chemistry data assimilation support by targeted observations

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The general problem:
Chemistry initial values are insufficient for optimisation. If so, how to identify the parameters to be optimised?

Specific problem:
Atmospheric chemical modelling includes O(100) chemical parameters per grid point as prognostic state variables. Emission rates are insufficiently well known, while exerting a high influence on the model evolution. Emission rate optimisation is as justified to be corrected by data assimilation as initial values (in stark contrast to meteorological and oceanic data assimilation).

For an optimal observation network design two central questions must be answered: 1. Which chemical constituents should be observed where and with preference? And 2. Is the observation system sensitive to both initial value and emission rate optimisation?

We need to know precisely, to find optimal sustainable and cost-efficient control strategies.

How can the observation configuration be optimized?
Or: what should be observed with preference?

Photochemical ozone production as a key process
Is frequently observed NOx always the controlling key to ozone production and analysis? And consequently, its observation the key to better forecast?

Identifying the principal sensitivities
Basic O3 Regional Atm. Chemistry Mechanism

Some mathematical background

How can the observation configuration be optimized?

Given CTM (here RAMC and EURAD-IM) acting as lin. model operator,

\[
\frac{\partial X}{\partial t} = \mathbf{A} X + \mathbf{B} U + \mathbf{D} \text{ for } t \in [0, \tau]
\]

For this find maximal eigenvectors as observation operators, \( \mathbf{N} \), which configure observations.

1. Berliner et al. (1998) Statistical design: “Minimise” the analysis error covariance matrix \( \mathbf{A} \) say, via trace:

\[
\text{min} \quad \text{tr} \left( \mathbf{A}^T \mathbf{A} \right)
\]

For this find maximal eigenvectors as observation operators, \( \mathbf{N} \), which configure observations.

2. Palmer (1999) Singular vector analysis:

Observational \( \mathbf{SV} \) configuration

Is the information needed available?
Location observation impact assessment on parameter optimisation by Ensemble Kalman Smoother

We seek to infer normalised sensitivity maps, which exhibit the control capacity of observations on parameters to be optimised: here emission rates vs. initial values.

Extended model with emission rates:

\[
\begin{align*}
\frac{\partial X}{\partial t} & = \mathbf{A} X + \mathbf{B} U + \mathbf{D} \text{ for } t \in [0, \tau] \\
\mathbf{A} & = \begin{bmatrix} \mathbf{A}_1 & \mathbf{A}_2 \end{bmatrix}, \mathbf{B} = \begin{bmatrix} \mathbf{B}_1 \\ \mathbf{0} \end{bmatrix} \text{ and } \mathbf{D} = \begin{bmatrix} \mathbf{D}_1 \\ \mathbf{0} \end{bmatrix}
\end{align*}
\]

Typically, there is no direct observation for emissions.

\[
\delta \mathbf{y} = \left( \mathbf{d}_n \right) \Rightarrow \text{inferred}
\]

Is the information needed available?

Exhibiting the control capacity of observations on parameters to be optimised

Infer normalised sensitivity maps for here emission rates and initial values.

Calculate the observability Gramian matrix (control theory) by forward and adjoint model M, observation operators \( \mathbf{H} \), and observation error covariance matrix.

\[
\mathbf{H}^T \mathbf{H} \left( \mathbf{H} \mathbf{H}^T \right)^{-1} \text{ or } \mathbf{H}^T \mathbf{H} \mathbf{K} \text{ or } \mathbf{H}^T \mathbf{H} \mathbf{H}^T \mathbf{K} \mathbf{H}^T
\]

Singular vectors for initial state and emission sensitivity

Arrive at a Degree of Freedom for Signal matrix (scaled forecast – analysis error covariance matrix from KS)

\[
\mathbf{p} = \mathbf{C} = \left( \mathbf{C} \right) \Rightarrow \mathbf{t} = \left[ \mathbf{C} \right] = \left( \mathbf{t} \right)
\]

Separate singular vector sections initial values, emission rates

Conclusions:
For both emission rate and initial value optimisation, singular vectors can be applied to determine the optimal placement for observations and to quantify which chemical compounds have to be observed with preference. With the Kalman smoother, a quantitative assessment method on the efficiency of observation configurations is devised based on singular value decomposition in order to evaluate normalized sensitivities to of initial values and emission rates.

References:
Wu, X. et al. (2017), GMD, in review.

Where should be observed?
Where is it important to observe for O3 prediction?
Example of maximal sensitivity contours of SV for
• emission rates (red) for flight,
• HCHO initial values (black)

19. Oct. 2008, 14.00 h, 15.20 h + at for final location,

References:
Wu, X. et al. (2017), GMD, in review.