Inversion of short lived pollutants in the global atmosphere using remote sensing data

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Outline

1. Objective
2. Glyoxal
3. Inverse Modeling
   - 4DVAR versus 3DVAR
4. TM5
5. Zooming
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Objective

- Better estimate of global glyoxal fluxes from various local sources
- For the first time using Tropomi satellite data in TM5
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→ Short lifetime requires high resolution (model and observations)
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  - 4DVAR approach versus Data Assimilation
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- For the first time using Tropomi satellite data in TM5
  \(\rightarrow\) Short lifetime requires high resolution (model and observations)
  \(\rightarrow\) 4DVAR approach versus Data Assimilation
  \(\rightarrow\) Multiple species influence one another
Glyoxal

- Smallest dicarbonyl (CHOCHO)
- Formed by oxidation of hydrocarbons
- Mostly ($\approx 70\%^1$) natural origin
- Sinks:
  - photolysis ($63\%^1$)
  - OH ($23\%^1$)
  - wet/dry deposition ($8\%/6\%^1$)
  - Aerosol formation (??)
- Life time: $\approx 1.3$ h in the sun$^2$, global mean 2.5 h to 3 h$^1,3$

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$^1$Myriokefalitakis et al. 2008, ACP
$^2$Volkamer et al. 2005, GRL
$^3$Fu et al. 2008, JGR; Stavrakou et al. 2009, ACP
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Glyoxal Inverse Modeling

4DVAR vs DA

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Glyoxal observations

GOME2A Glyoxal VCs: 2005-2014

- Elevated levels near...
  - Biomass burning
  - Anthropogenic emissions
  - Dense vegetation

Maps: Leonardo Alvarado (personal communication)
Glyoxal observations

GOME2A Glyoxal VCs: 2005-2014

- Elevated levels near...
  - Biomass burning
  - Anthropogenic emissions
  - Dense vegetation
  - Over the remote ocean(!)

Maps: Leonardo Alvarado (personal communication)
Glyoxal over the ocean

- Observed in multiple satellite data sets
- Verified with ship based MAX-DOAS
- Close to upwelling areas and above areas with high phytoplankton concentrations, but not always
- Cannot be reproduced with models

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Glyoxal over the ocean - Modeling

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Images: Myriokefalitakis et al. 2008, ACP
Glyoxal over the ocean - Suggested Explanations

- Concentration peaks in afternoon $\rightarrow$ likely photochemistry
  - Unknown local source?
  - Long range transport of acetylene and acetone?
- Uptake, transport and re-release via unknown secondary organic aerosol?
- Outflow of longer lived continental isoprene $\rightarrow$ does not fit patterns
Inverse Modeling

Find the state that minimizes the difference between a set of observations and a model that links the state to the observations.
Inverse Modeling - Mathematical description

- Forward model $\mathbf{F}$ with parameters $\vec{p}$ links state $\vec{x}$ to observation $\vec{y}$
  \[ \vec{y} = \mathbf{F}(\vec{x}, \vec{p}) \]

- Inversion (of $\mathbf{F}$): get cause $\vec{x}$ from observation $\vec{y}$
Inverse Modeling - Mathematical description

- Forward model $\mathbf{F}$ with parameters $\mathbf{p}$ links state $\mathbf{x}$ to observation $\mathbf{y}$

$$\mathbf{y} = \mathbf{F}(\mathbf{x}, \mathbf{p}) + \mathbf{\varepsilon}_O$$

with observational error $\mathbf{\varepsilon}_O$ (error of measurements, model, and parameters)

- Inversion (of $\mathbf{F}$): get cause $\mathbf{x}$ from observation $\mathbf{y}$
Inverse Modeling - Cost function

- Least squares approach
- Assume a priori state $\vec{x}_A$
- Error covariance matrices $S_O$ and $S_A$
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$$J(\vec{x}) = \begin{array}{c} \text{state-a priori error} \\ \text{obs-model error} \end{array}$$

Cost = \begin{array}{c} \text{state-a priori error} \\ \text{obs-model error} \end{array}$$
Inverse Modeling - Cost function

- Least squares approach
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$$J(\vec{x}) = (\vec{x} - \vec{x}_A)^T S_A^{-1} (\vec{x} - \vec{x}_A) +$$

$$\text{Cost} = \frac{(\text{state-a priori})^2}{\text{error}_{apri}} +$$
Inverse Modeling - Cost function

- Least squares approach
- Assume a priori state $\vec{x}_A$
- Error covariance matrices $S_O$ and $S_A$

$$J(\vec{x}) = (\vec{x} - \vec{x}_A)^T S_A^{-1} (\vec{x} - \vec{x}_A) + (\vec{y} - F(\vec{x}))^T S_O^{-1} (\vec{y} - F(\vec{x}))$$

Cost = \frac{(\text{state-a priori})^2}{\text{error}_{apri}} + \frac{(\text{obs-model})^2}{\text{error}_{obs}}$$
Concrete applications to evaluate the cost function for given observations
Assimilate data at a single point in time, after a fixed time step.

- Optimizes only the result and only in space (but not time).
  - Optimizer does not need forward model.
Assimilation - 4DVAR

- Assimilate data \textit{spread} over the time step, \textit{back} to its starting point
- Optimizes in space \textit{and} time
3D, global CTM
- Well established and documented
- Handles different in situ and satellite datasets
- Capable of 4DVAR or 3DVAR (CTDAS)
- Zooming
Aim: Model chemistry on arbitrarily large domain
Zooming

- **Aim:** Model chemistry on arbitrarily large domain
- **Problems:**
  - High resolution $\rightarrow$ high computational demands
  - Low resolution $\rightarrow$ bad representation of local processes
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    - Numerical Dilution
    - Non-linear chemistry
    - Transport
    $\rightarrow$ All especially relevant for short lived species
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- High resolution $\rightarrow$ high computational demands
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Solution: Use low resolution where possible and high resolution only where necessary
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Image: Bergamaschi et al. 2005, ACP
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Zooming - Pros and Cons

- Straightforward: increase resolution in region of interest
- Results close to full high resolution run and much faster

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Zooming - Pros and Cons

- Straightforward: increase resolution in region of interest
  - Results close to full high resolution run and much faster
  - Still limited by grid box size

Image: Bergamaschi et al. 2005, ACP
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- Increase zooming capabilities of TM5 to at least $0.5^\circ \times 0.5^\circ$
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- Implement inversion schemes for CHOCHO, HCHO and NO$_2$
Glyoxal as short-lived tracer with unknown fluxes

Inverse modeling with focus on 3DVAR and 4DVAR

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Extend to handle multi-tracer inversion
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- Compare results to CTDAS
Acknowledgments

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Thank you!

... to be continued ...