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

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Outline

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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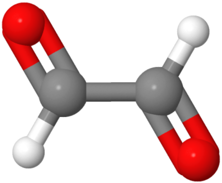
→ Short lifetime requires high resolution (model and observations)

→ 4DVAR approach versus Data Assimilation

→ 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]

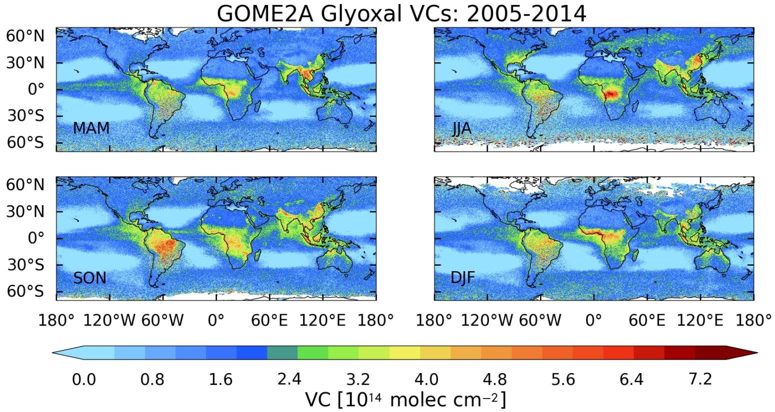


[1] Myriokefalitakis et al. 2008, ACP

[2] Volkamer et al. 2005, GRL

[3] Fu et al. 2008, JGR; Stavrakou et al. 2009, ACP

Glyoxal observations



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

Maps: Leonardo Alvarado (personal communication)

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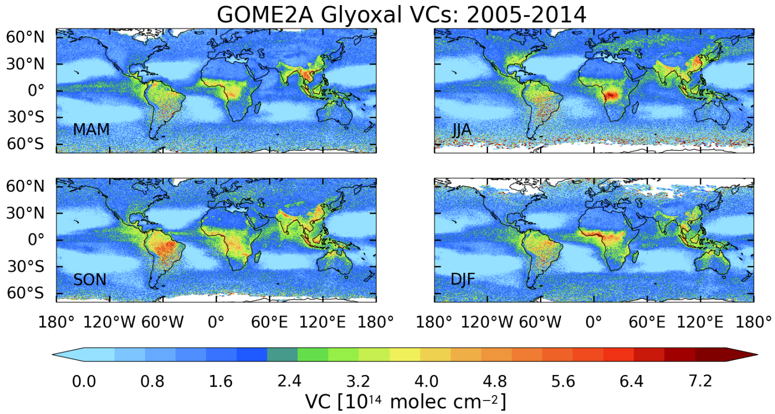

- Elevated levels near...
  - Biomass burning
  - Anthropogenic emissions
  - Dense vegetation
  - Over the remote ocean(!)

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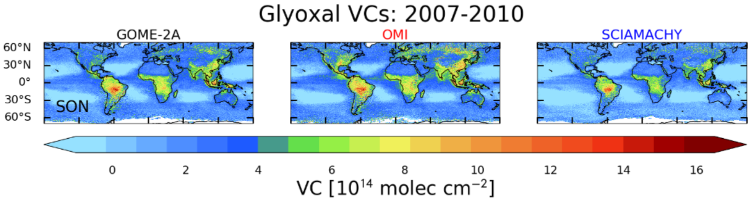
Glyoxal over the ocean



- 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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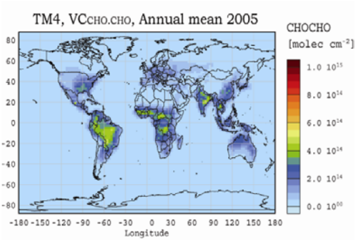
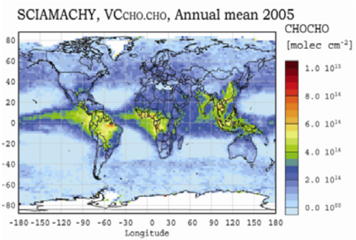
Glyoxal over the ocean - Modeling





Images: Myriokefalitakis et al. 2008, ACP

Glyoxal over the ocean - Suggested Explanations

- Concentration peaks in afternoon → 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 → 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 **F** with parameters $\vec{p}$ links state $\vec{x}$ to observation $\vec{y}$

$$\vec{y} = \mathbf{F}(\vec{x}, \vec{p})$$

- Inversion (of **F**): get cause $\vec{x}$ from observation $\vec{y}$

Inverse Modeling - Mathematical description

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

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

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

- Inversion (of **F**): get cause $\vec{x}$ from observation $\vec{y}$

Inverse Modeling - Cost function

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

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$$J(\vec{x}) = (\vec{x} - \vec{x}_A)^T \mathbf{S_A^{-1}} (\vec{x} - \vec{x}_A) \quad +$$

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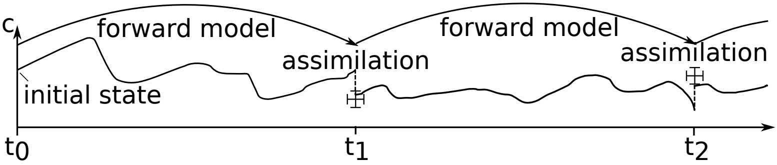
$$J(\vec{x}) = (\vec{x} - \vec{x}_A)^T \mathbf{S_A^{-1}} (\vec{x} - \vec{x}_A) \quad + (\vec{y} - \mathbf{F}(\vec{x}))^T \mathbf{S_O^{-1}} (\vec{y} - \mathbf{F}(\vec{x}))$$

$$\text{Cost} = \frac{(\text{state-a priori})^2}{\text{error}_{\text{apri}}} \quad + \frac{(\text{obs-model})^2}{\text{error}_{\text{obs}}}$$

Assimilation

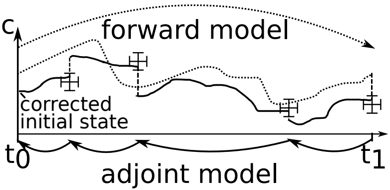
Concrete applications to evaluate the cost function for given observations

Assimilation - 3DVAR



- 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 *spread* over the time step, *back* to its starting point
- Optimizes in space *and* time

TM5

- 3D, global CTM
- Well established and documented
- Handles different in situ and satellite datasets
- Capable of 4DVAR or 3DVAR (CTDAS)
- Zooming

Zooming

- Aim: Model chemistry on arbitrarily large domain

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    - Numerical Dilution
    - Non-linear chemistry
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    $\rightarrow$ All especially relevant for short lived species
- Solution: Use low resolution where possible and high resolution only where necessary

Zooming - Pros and Cons

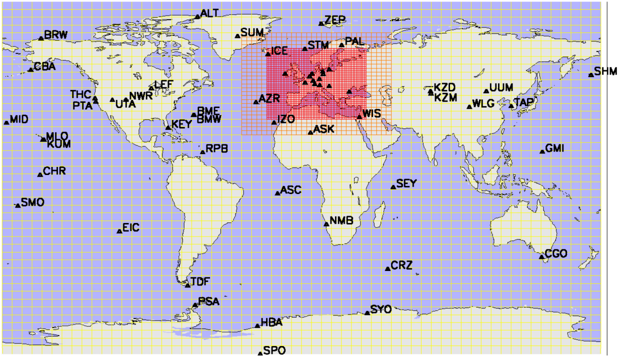

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Image: Bergamaschi et al. 2005, ACP

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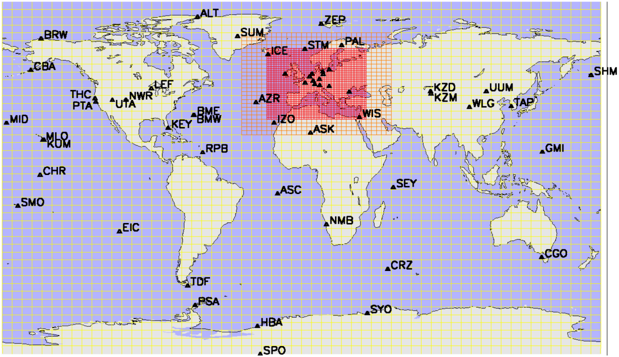

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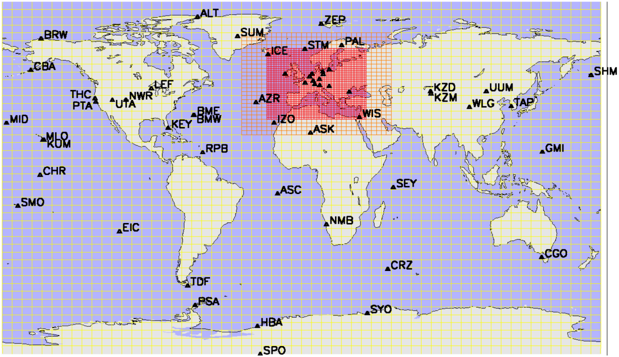

- Straightforward: increase resolution in region of interest
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- – Still limited by grid box size

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- Compare results to CTDAS

Acknowledgments

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- Thank you to the LAMOS group, especially Nikos and Mihalis.
- Special thanks to Leonardo Alvarado for the quick provision of the glyoxal maps.

Thank you!

... to be continued ...