Probing the relationship between formaldehyde column concentrations and soil moisture using mixed models and attribution analysis

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Using formaldehyde as a proxy of isoprene emissions

Volatile Organic Compounds (VOC) are oxidized to produce Formaldehyde (HCHO). On ~100-km scale, HCHO is mainly sensitive to isoprene emissions (Marais et al., 2012; Stavrakou et al., 2018).

Among biogenic volatile organic compound (BVOCs) emitted by vegetation, isoprene is the most abundant (Guenther et al., 2012).
Isoprene emissions and water stress

Why do we care about this relationship?

Sunny, warm, calm days

ANTHROPOGENIC EMISSIONS

NOx

OZONE POLLUTION

Effect on BVOC drivers
- temperature, precipitation, solar radiation, soil moisture

BVOCs

Isoprene emissions affect levels of ozone, methane and particulate matter (Pacifico et al., 2009). Climate change may alter isoprene emissions by modifying the occurrence and intensity of severe stresses that influence plant functioning (Niinemets, 2010).
Isoprene emissions and response to abiotic factors

Radiation, temperature and water availability

Radiation and temperature dependence

Water stress dependence

Well established relationship

Zimmer et al. (2000)

Peñuelas and Staudt (2010)

Under water stress, emissions decrease or increase?

Niinemets (2010)

Peñuelas and Staudt (2010)

No. papers reporting BVOC emission increase, decrease or no-change in response to drought

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## Selected observational global datasets

<table>
<thead>
<tr>
<th>Variable and dataset</th>
<th>Period</th>
<th>Resolution</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>OMI-HCHO (vQA4ECV, L3)</td>
<td>2005–2016</td>
<td>0.25°</td>
<td>De Smedt et al. (2018)</td>
</tr>
<tr>
<td>CRU Temperature (v4.03)</td>
<td>1901–2018</td>
<td>0.50°</td>
<td>Univ. East Anglia CRU (2020)</td>
</tr>
<tr>
<td>CRU Precipitation (v4.03)</td>
<td>1901–2018</td>
<td>0.50°</td>
<td></td>
</tr>
<tr>
<td>Standardised Precipitation-Evapotranspiration Index (SPEI, v2.6)</td>
<td>1901–2018</td>
<td>0.50°</td>
<td>Vicente-Serrano et al., 2010</td>
</tr>
<tr>
<td>GLEAM Root-Zone Soil Moisture (v3.3b)</td>
<td>1978–2018</td>
<td>0.25°</td>
<td>Martens et al. (2017)</td>
</tr>
<tr>
<td>Copernicus Leaf Area Index (LAI)</td>
<td>2005–2017</td>
<td>0.50°</td>
<td>Verger et al. (2015)</td>
</tr>
<tr>
<td>MODIS C6 Aerosol Optical Depth (AOD) (L3, Terra and Aqua)</td>
<td>2002–2017</td>
<td>0.05°</td>
<td>Levy et al. (2013)</td>
</tr>
<tr>
<td>FLUXCOM Latent Heat</td>
<td>2001–2015</td>
<td>0.50°</td>
<td>Jung et al. (2019)</td>
</tr>
</tbody>
</table>

All data re-mapped to a 2.5° horizontal resolution

Period for analysis: 2005–2016 → Availability of OMI-HCHO observations

Color legend:  
- **Aquiring**
- **Discarded**

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Linear mixed-effects (LME) model

How to deal with non-independence in the data?

Both spatial and temporal levels of dependence in the dataset

Global dataset

Time series in each pixel

ALTERNATIVE 1
By applying a simple linear regression at each pixel, the model is noisy and does not use all information

Outcome

Predictor

ALTERNATIVE 2
By aggregating data at the pixel level, the model is less noisy but some information is lost

Linear mixed-effects models are a trade-off between these two alternatives that account for both **fixed** (variation explained by explanatory variables) and **random** (not explained by explanatory var.) **effects**
Linear mixed-effects model

Random intercept model

\[ Y_{HCHO} = \underbrace{\alpha + \beta_1 X_1 + \cdots + \beta_q X_q}_{\text{fixed part}} + \underbrace{\text{random part}}_{\text{Site-level variability}} + \underbrace{\epsilon}_{\text{Residuals}} \]

In the fixed-effect part, the contribution of the explanatory variables and their interactions is accounted and described using linear regression models.

The random intercept model assumes that the variation around the intercept is normally distributed with a certain variance.
Linear annual trend in formaldehyde

OMI-HCHO version QA4ECV, Level 3 (period: 2005–2016)

By applying a LME model, HCHO does not show an overall trend at the global scale, while robust trends emerge at the regional scale.
**LME model and temporal contribution analysis**

**Regional scale: Australia**

- Accounting for only climatic drivers, the LME model (blue line) does not reproduce the observed regional trend in HCHO (black line).
  \[ \Rightarrow \text{Need to add other explanatory variables!} \]

- When keeping constant the contribution over years of one explanatory variable at-a-time (red line), SPEI and root-zone soil moisture show an important contribution.
Conclusions and perspectives

- Formaldehyde column concentrations show no overall trend at the global scale, but robust trends at the regional scale.
- Including only climatic drivers, the linear mixed-effects model explains more than 50% of the observed variance of formaldehyde. However, to correctly reproduce the observed trend, some information is still missing (as observed for Australia).
- Over Australia, the Standardised Precipitation-Evapotranspiration Index (SPEI) and the root-zone soil moisture show important temporal contributions.

Next steps
Include as explanatory variables:

- Leaf Area Index (LAI) to account for trends in biomass;
- Burned fraction to account for trends in wildfires, which are an important source of formaldehyde;
- Aerosol Optical Depth to account for anthropogenic sources of formaldehyde.

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References

De Smedt et al.: Algorithm theoretical baseline for formaldehyde retrievals from S5P TROPOMI and from the QA4ECV project. Atmospheric Measurement Techniques, 2018.


