Anthropogenic VOC speciation in emission inventories: a method for improvement and evaluation

Erika von Schneidemesser, Ariela Danigola, Claire Granier, Paul S. Monks, and Kathy Law
VOCs, CO, & urban areas

• VOCs are an important contributor to the formation of ozone and other secondary pollutants
• Speciated VOCs are not well represented in emission inventories
• Focus here is on urban areas and therefore predominantly anthropogenic NMHCs
• CO is a combustion tracer can facilitate comparisons between cities

![Graph showing the mixing ratio of various compounds](chart.png)
VOC concentrations show significant variation among cities;

VOC:CO ratios show significant similarity among cities
von Schneidemesser, et al.

Annex 1 countries

Non-Annex 1 countries

alkanes | alkenes | aromatics

Annex 1 countries

Atm Env (2010)
indicates similarity of emission sources

VOC:CO similarity among urban areas
What about changes in emission over time?
VOC and CO emissions have declined over the past decade in London.
The VOC:CO ratios stayed constant.
How do the ratios from measurements compare to the ratios in the emission inventories?
Anthropogenic Emissions

ACCMIP

- decadal emissions period = 1850-2100
- developed in support of the IPCC simulations (Lamarque et al., ACP, 2010)

http://www.iiasa.ac.at/webapps/ind/RS/10-0210

MACC4 CITIZEN PROJECT

VOC Speciation of Anthropogenic Emissions in MACCity dataset:

- based on ACCMIP
- yearly emissions
- period = 1990-2010 (linear interpolation)
- MACC4 CITIZEN PROJECT (emissions developed for Chemistry and Climate Model)
- MACCIP

R is obtained from the RETRO database for the year 2000 for all the years for each grid cell; remains constant for all years.

[Emission VOC\(x\)] = [Total VOC emissions] \(R\)

Methodology:

- based on a speciation developed by TNO (Utrecht, The Netherlands)
- both available in the ECAD website: http://eccad.sedoo.fr

VOC Speciation of Anthropogenic Emissions in MACCity dataset:

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VOC&CO observations by regions

**Asia**
- 28 US cities (5 week summer measurements August 8-2006)
- 43 Chinese cities (January & February 2001)
- Lagos, Nigeria
- Athen, Greece (7-8am June 1993, May 8 July 1994)
- Tokyo, Japan (September 2002-August 2003)
- Hong Kong, China (1999)
- Karachi, Pakistan (December 12 1998-January 11 1999)
- Ahmedabad, India (January 8 February 2001)
VOC:CO ratio
emission inventory and observational data

Ethane
Propane
Butanes
Pentanes
Ethene
Propene
Ethyne
Benzene
Toluene
Xylenes

Marylebone Road observational data
model emission inventory data

London, England
How can we use this information to evaluate VOC speciation in the emission inventories?
\[
\text{ave} = \text{CO CO} \times \left( \frac{\text{CO}}{\text{CO}^{\text{VOC}}} \right)
\]

Methodology for Improved VOC Specification:

1. New VOC Emission Inventory
2. VOC:CO Ratios
3. Countries (by region, Annex I), Developing Countries
4. CO Emission Inventory
5. Observed Data

Countries:
- North America
- Europe
- Latin America
- Africa
- Southeast Asia

Ratios:
- VOC:CO Ratios

Min / Avg / Max VOC:CO Ratios
Apply the ratio to urban areas, defined by population thresholds.
Max, min, and avg VOC:CO ratios were applied to estimate a new speciation.
a. MIN: Minimum ratio new VOC speciation
b. AVE: Average ratio new VOC speciation
c. MAX: Maximum ratio new VOC speciation
d. STD: Base case (previous VOC speciation)

Year Run=2005 (2004 spin-up)

- 28 vertical levels up to 30 km
- T63 spatial resolution 1.8° x 1.8°
- Driven by offline meteorology
- Full code freely available online
- Emmens et al., Geosci. Model Dev., 2010

MOZART

Model for Ozone and Related Chemical Tracers

Version 4: Community Chemistry-Chemistry-Transport

= model

run with the MOZART 4 model.

Year long runs using the test VOC speciations were
but how does this compare with observations?

Max-Std runs show significant differences, globally...
Trinidad Head (USA)

Ethane (ppb)

CO (ppm)

Propane (ppb)

Mace Head (Ireland)

O3 (ppb)

CO (ppm)

Ethane (ppb)


Observations (2005)
Beijing, China (obs. Jan. 2001)

<table>
<thead>
<tr>
<th>Ethane (ppb)</th>
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Ahmedabad, India (obs. 2002)

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Beijing, China (obs. Jan. 2001)
Conclusions

- Number of stations performing continuous/longer-term monitoring and reporting of individual VOCs (and CO) is lacking.
- Monitoring of speciated VOCs and CO could improve model results and the understanding of the impact of VOCs on air quality.
- Based on available VOC & CO data, the relative amounts of VOC species and CO in the emission inventory could be improved.
- This sensitivity study on changing the VOC speciation in the emission inventory shows that speciation can affect CO concentrations.
- Production of CO from improved VOC speciation is increased, but does not contribute enough to resolve the deficit in CO concentrations.
- There is a need to improve the VOC speciation in emission inventories and know more about VOC speciation from observations.
- Monitoring of speciated VOCs and CO could improve model results.
- Number of stations performing continuous/longer-term monitoring is lacking.
- Monitoring of individual VOCs (and CO) is lacking.
Thank you!

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