Comparing measurements and emission inventory data for NMVOCs in urban areas
(a GEIA NMVOCs Working Group activity)

Erika von Schneidemesser (evs@iass-potsdam.de)
Brian McDonald, Shelby Tisinai, Monica Crippa, Gregory Frost, Hugo Denier van der Gon, Leyang Feng, Ganlin Huang, Greet Janssens-Maenhout, Chang-Feng Ou-Yang, Jia-Lin Wang, Steven Smith, and the GEIA NMVOC Working Group Members
Founded in 1990, GEIA is a community initiative that builds bridges between environmental science and policy, by bringing together people, data, and tools to create and communicate the highest quality information about emissions.

Core Activities

Promoting broad and consistent access to emissions information

www.geiacenter.org
Progress in GEIA Working Groups

China Emissions WG
Contacts: Kebin He, Qiang Zhang, Yuxuan Wang
• Improving scientific basis for Chinese emissions
• Sharing results between Chinese research groups
• Publishing in ACP’s East Asian Emissions Assessment
  ➢ 36 papers published since 2014!

VOC Emissions WG
Contacts: Erika von Schneidemesser, Hugo Denier van der Gon
• Improving global understanding of VOC emissions
• Leveraging on-going inventory development, measurements, modelling
• Starting evaluation of megacity VOC emissions

Latin America/Caribbean (LAC) Emissions WG
Contacts: Nicolas Huneeus, Laura Dawidowski, Néstor Rojas
• Developing and evaluating LAC-specific emissions information and harmonized national emissions inventories
• Building LAC emissions expert community
• Multinational LAC collaboration has recently been funded

http://www.geiacenter.org/analysis/working-groups
Initial proposal
• Review of measurement-EI comparisons (with information on sector allocation)

Scope
• focus on anthropogenic emissions; leave out biogenic emissions
• spatial variability/regional comparisons
• compare to a ‘reference’ value (EI), e.g. EDGAR
• initial focus on urban areas
• **compare the speciation using emission ratios**, either for urban areas as a whole, or where possible by sector
• **confirm/falsify dominant source sector contributions** in urban areas globally -> does this agree or disagree with the emission inventories (using a global inventory as a basis, e.g. EDGAR)
• to provide guidance on **key species** for measurements/monitoring
• **evaluate differences between cities, countries, regions** (possible patterns, generalizable?)
• identify the most pressing **data gaps** by continent / region [acknowledging that for a continent where no measurements are available the need is different from one where already substantial data is but that would still need significant refining or broadening]
Warneke et al 2007

Figure 8. Comparison of the measured emission ratios with CO with an anthropogenic emissions database based on EPA NEI-99 data that is used in various air quality forecast models. Each data point represents one compound, and the solid lines are linear fits through the data. The grey shaded area shows an agreement within a factor of two.
Fig. 3. Relationship between mixing ratios of n-hexane and toluene in the same format as Fig. 1. The “best” average molar ratios of n-hexane to toluene for three data sets are taken as the slope of the linear-least-squares fit to the measurements, with the y-intercept of the line forced through zero. The geometric mean ratio of the observations was taken as the “best” average ratio for the 71 US cities data and Tokyo.
Basis

- Warneke et al 2007
- Parrish et al 2009
- von Schneidemesser et al 2010
Basis

- Warneke et al 2007
- Parrish et al 2009
- von Schneidemesser et al 2010
- Borbon et al 2013

Figure 10. Comparison of the measured emission ratio relative to (a, c, d, f) CO and (b, e) acetylene to the ones in the anthropogenic VOC emission database currently used in Los Angeles and Paris (see text for details). Abbreviations are as follows: c1, methanol; c2, acetaldehyde; c3, benzaldehyde; h1, 2-methylpentane; h2, 2,3-dimethylpentane; h3, methylcyclohexane; h4, n-heptane; h5, 3-methylhexane; h6, n-nonane; h7, n-decane.
Base data - obs

-primarily short-term campaign data
-differing years and months
-mostly from previous work for initial scoping

-further data from WG members and others that would be included as the work develops
-additional possibilities with long-term monitoring data
Global emission inventory datasets:

- **EDGAR v4.3.2**
- **CEDS**
Initial conditions

<table>
<thead>
<tr>
<th>EI Compound (Group)</th>
<th>Obs Compound(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethane</td>
<td>ethane</td>
</tr>
<tr>
<td>Propane</td>
<td>propane</td>
</tr>
<tr>
<td>Butanes</td>
<td>nbutane + ibutane</td>
</tr>
<tr>
<td>Pentanes</td>
<td>ipentane + npentane</td>
</tr>
<tr>
<td>Hexanes and higher</td>
<td>nhexane + nheptane + noctane</td>
</tr>
<tr>
<td>Ethene</td>
<td>Ethene</td>
</tr>
<tr>
<td>Propene</td>
<td>Propene</td>
</tr>
<tr>
<td>Ethyne</td>
<td>ethyne</td>
</tr>
<tr>
<td>Other alk(adi)enes/alkynes</td>
<td>1butene</td>
</tr>
<tr>
<td>Benzene</td>
<td>benzene</td>
</tr>
<tr>
<td>Methylbenzene</td>
<td>toluene</td>
</tr>
<tr>
<td>Dimethylbenzenes</td>
<td>oxylene + mpxylene</td>
</tr>
<tr>
<td>Other aromatics</td>
<td>ethylbenzene</td>
</tr>
</tbody>
</table>

- All ratios VOC$_i$/acetylene
- Match year & month between obs & EI
- Total emissions, no sector breakdown
- No accounting for photochemical age / assume relatively fresh emissions for urban obs
- Extract grid cells (1, 9, 25 cells) from the urban areas where we have obs data
Initial Results –
Obs vs EI – VOCi/acetylene Ratios
Initial Results – Obs vs EI – VOCi/acetylene Ratios

Propene

Toluene

EI ratio vs Obs ratio for Propene and Toluene. The graphs show the Obs/PI ratios with various data points representing different countries and emission models.
• There is significantly more variability in the EI ratios than in the obs
  -> where is this coming from? Specific sectors?

Next Steps
• Focus on 2-4 cities with significant measurements (e.g., LA, NY, London, Beijing, Taiwan, Mexico City)
• Compare national to global EI -> how similar?
• Evaluate different denominators for the ratios; influence of photochemical age
• Eventually, expand obs data
London – obs vs EI (yr 2000 only)
London – obs vs EI (yr 2000 only)
London – obs vs EI (yr 2000 only)
London – obs vs EIs
2000-2008 annual average values
London – obs vs EDGAR urban cells
2000-2008 annual average values
UK NAEI vs EDGAR UK National Total

![Graph showing comparison between UK NAEI and EDGAR UK National Total emissions for various compounds.](image-url)
Difference between accounting for photochemical age and not

Los Angeles (2010)

VOC / Ethyne (g / g)

- Ethane
- Propane
- Butanes
- Pentanes
- Hexane
- Ethene
- Propene
- Other Alkenes
- Benzene
- Toluene
- Xylenes
- TMB

Photochemical Age Method

Ambient Ratio
Difference between accounting for photochemical age and not

New York City (2004)

- Ethane
- Propane
- Butanes
- Pentanes
- Hexane
- Ethene
- Propene
- Other Alkenes
- Benzene
- Toluene
- Xylenes
- TMB

VOC / Ethyne (g / g)

- Photochemical Age Method
- Ambient Ratio
Los Angeles – accounting for photochemical age

![Graph showing the relationship between EDGAR VOC/Ethylene and Top-Down VOC/Ethylene for Los Angeles (2010). The graph includes data points for various hydrocarbons and a regression line with an R² value of 0.00.]
New York – accounting for photochemical age

![Graph showing the ratio of EDGAR VOC to Ethyne in New York City (2004). The graph includes points for various compounds such as Xylenes, Toluene, Butanes, Hexane, Propane, Ethene, Benzene, Ethane, Other Alkenes, Propano, and TMB. The coefficient of determination, $r^2 = 0.07$, is indicated.]
Summary

• Initial scoping to synthesize / review measurement-EI comparison
  • using a comparable (global) baseline EI (EDGAR)
  • using emission ratios, currently VOC:acetylene
  • in urban areas

• Generally finding more variability in the EI ratios than in the obs
• LA, NY, London show large differences between the obs & various EI ratios
• National total UK NAEI and EDGAR EIs also show differences in the ratios
• Ambient ratios trend to be lower than those accounting for photochemical age for LA, NY

Next steps

• Evaluate different denominators for the ratios
• More accounting for photochemical age
• Expand city analysis to include a couple more cities, eventually expand obs data

Thank you for your attention! Thoughts? Questions? Ideas?