Evaluation of simulated SOA in Seoul during KORUS-AQ 2016

Yujin Oak¹, Rokjin Park¹, Duseong Jo², and KORUS-AQ team

¹Seoul National University
²University of Colorado Boulder

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Major components of PM$_{2.5}$ in observations

- Black carbon
- Ammonium
- Nitrate
- Sulfate
- Organic (POA+SOA)

Zhang et al., 2007
NIER and NASA, 2017
## Modeling secondary organic aerosols

parent hydrocarbons + OH, O₃, NO₃ →→→→ γ SOA \( (\gamma : \text{SOA yield}) \)

<table>
<thead>
<tr>
<th>SOA scheme</th>
<th>parent HC</th>
<th>VBS</th>
<th>SOA aging</th>
<th>SVPOA</th>
<th>updated yield</th>
<th>additional description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pye</td>
<td>isoprene, terpenes, aromatics</td>
<td>○</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>• GC default (complex) SOA scheme</td>
</tr>
<tr>
<td>(Pye et al., 2010)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Simple</td>
<td>SOAP (lumped)</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>×</td>
<td>• SOAP → SOAS ( (\tau_{\text{SOAP}}=1\text{day}) )</td>
</tr>
<tr>
<td>(Hodzic and Jimenez, 2011; Hayes et al., 2015; Shrivastava et al., 2017)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>• SOAP directly emitted proportional to CO ( \frac{\text{SOAP}<em>{\text{fossil}}}{\text{CO}}=0.069 \text{ g/g}, \frac{\text{SOAP}</em>{\text{biomass}}}{\text{CO}}=0.013 \text{ g/g} )</td>
</tr>
<tr>
<td>Hodzic</td>
<td>isoprene, terpenes, aromatics, S/IVOCs</td>
<td>○</td>
<td>×</td>
<td>×</td>
<td>○</td>
<td>• stronger production (wall-corrected yields)</td>
</tr>
<tr>
<td>(Hodzic et al., 2016)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>• faster and additional removal (updated Henry’s law coeff., photolysis, oxidation)</td>
</tr>
<tr>
<td>Jo</td>
<td>isoprene, terpenes, aromatics, S/IVOCs</td>
<td>○</td>
<td>○</td>
<td>○</td>
<td>×</td>
<td>• chemical aging of aromatic SOA</td>
</tr>
<tr>
<td>(Jo et al., 2013)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>• semi-volatile POA with VBS (further oxidizes POA)</td>
</tr>
</tbody>
</table>
## Model configuration and observations

### GEOS-Chem v12 (v10 for Jo SOA scheme)

**Simulation period:** 2016/05/01 – 2016/06/10

<table>
<thead>
<tr>
<th><strong>Horizontal resolution</strong></th>
<th><strong>Meteorology</strong></th>
<th><strong>Biogenic emissions</strong></th>
<th><strong>Anthropogenic emissions</strong></th>
<th><strong>Biomass Burning</strong></th>
<th><strong>PBL mixing</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>0.25° x 0.3125° (nested)</td>
<td>GEOS-FP</td>
<td>MEGAN v2.1</td>
<td>KORUS v2.0 (East Asia)</td>
<td>GFED4 (daily)</td>
<td>non-local mixing (VDIFF)</td>
</tr>
</tbody>
</table>

### Korea-US Air Quality field campaign (May–June 2016)

- International cooperative air quality monitoring campaign held in Korea
- Extensive **surface and airborne measurements** with high temporal resolutions conducted
- **Airborne measurements** (20 flights onboard DC-8 aircraft)
- **Ground measurements** at super sites

**KORUS-AQ Goals**

- Improve capability for satellite remote sensing of air quality
- Better understanding of the factors controlling air quality
- Test and improve model simulation of air quality

**Ground monitoring**

- It will continue to be the primary method for monitoring exposure.
- Coverage is limited.

**Satellites**

- Provide broad coverage, continuity
- But it needs reliable information on near-surface exposure.

**Airborne sampling**

- Provides critical view for evaluation strategies in connecting ground-based and satellite observations
- Short term

**Ground monitoring**

- Provide Air quality forecasting and warning service
- But it needs reliable information on emission inventory and so on.
Evaluation of simulated OA concentrations

Comparison with **airborne (DC-8)** observations over Seoul

![Graph comparing simulated OA concentrations with airborne observations over Seoul.](image)
Composition of observed (PMF) and simulated OA

**DC-8**
- OBS (Nault et al., 2018)
  - Primary (20-40%)
  - Secondary (60-80%)
- Pye
  - Primary
  - Secondary
- Simple
  - Primary
  - Secondary
- Hodzic
  - Primary
  - Secondary
- Jo
  - Primary
  - Secondary

**OBS (Kim et al., 2018)**
- Primary (20-40%)
- Secondary (60-80%)

**Ground**
- Primary (20-40%)
- Secondary (60-80%)
Evolution of OA with photochemical age

Nault et al., 2018
Evolution of OA with photochemical age

Correlation of OA with $O_x$

<table>
<thead>
<tr>
<th>Slope (R)</th>
<th>OBS</th>
<th>Pye</th>
<th>Simple</th>
<th>Hodzic</th>
<th>Jo</th>
</tr>
</thead>
<tbody>
<tr>
<td>OA</td>
<td>0.39 (0.67)</td>
<td>0.19 (0.38)</td>
<td>0.40 (0.33)</td>
<td>0.54 (0.62)</td>
<td>1.17 (0.44)</td>
</tr>
<tr>
<td>POA</td>
<td>-</td>
<td>0.14 (0.25)</td>
<td>0.15 (0.13)</td>
<td>0.14 (0.24)</td>
<td>0.08 (0.21)</td>
</tr>
<tr>
<td>SOA</td>
<td>-</td>
<td>0.06 (0.59)</td>
<td>0.27 (0.42)</td>
<td>0.44 (0.69)</td>
<td>1.13 (0.45)</td>
</tr>
</tbody>
</table>
Summary

- Pye and Simple schemes underestimate, and the Jo scheme overestimates observed OA concentrations, whereas the Hodzic scheme well-captures the observed vertical profile.
- Observations show that 20-40% of OA is primary and 60-80% is secondary.
- Pye and Simple overestimate the POA portion due to lack of SOA formation.
- Jo underestimates the POA portion and overestimates the SOA portion (especially aromatics) due to the simulation of SVPOA and aging.
- Hodzic shows increase in formation of SOA as photochemical age increases.
- High OA/O\textsubscript{x} ratio and correlation is shown in Hodzic, emphasizing the role of photochemical processes in OA formation.