Modelling Organic Aerosol in the EMEP MSC-W model – focus on primary organic aerosol (POA)

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EMEP MSC-W model

- Chemical transport model

- Flexible scale/input (local → global, HTAP)

- Flexible chemical scheme (CB4,CB5,EMEP,CRI,..)

- Several SOA schemes (VBS, semi-explicit, easy to change)

- Very CPU efficient – allows 100s years simulation

- Open source (www.emep.irt); Simpson et al., ACP; 2012

- Uses in several countries, e.g. EMEP4UK, EMEP4HR
EMEP (S)OA modelling:

Started 1998-ish
Still going st/w-rong
Still a horrendous subject

Tested Several SOA schemes (Kamens-type, a-K, VBS), made much use of measurements (e.g. levoglucosan, 14C), etc.

See Andersson-Sköld & Simpson, 2001(JGR), Simpson et al. 2007(JGR), Bergström et al., 2012, 2014(ACP), 2015(PhD), Genberg et al., 2011, 2013 (ACP), Denier van der Gon et al., 2015 (ACP)
SOA: horrendous subject (still!)

- OC<sub>bb</sub> OC from residential wood burning
- EC<sub>bb</sub> EC from residential wood burning
- OC<sub>ff</sub> OC from combustion of fossil fuel
- EC<sub>ff</sub> EC from combustion of fossil fuel
- OC<sub>pbs</sub> OC from fungal spores
- OC<sub>pbc</sub> OC from plant debris
- OC<sub>bsoa</sub> OC from biogenic sec. org. aerosols
- OC<sub>asoa</sub> OC from anthropogenic sec. org. aerosols

- OA modelling is unique in many ways
- e.g. presumed main sources (wood-burning, BVOC) are also those we know least about!
- .. and there may be ‘unknown’ sources too (diesel IVOC, diffuse VOC..)
Organic aerosol in Europe – estimate of sources

Winter (Nov-Apr)

Summer (May-Oct)

Wood burning dominates during winter!

Biogenic SOA (from unstressed vegetation)
Early lessons in organic aerosol (CARBOSOL project)

- First OA results not promising, e.g. Aveiro (Simpson et al., 2007)
- Incorrect conclusion: problems with model
Early lessons in organic aerosol (CARBOSOL project)

- Aveiro revisited, after use of levoglucosan-scaling (Simpson et al., 2007)
- Correct conclusion: problems with inventory (or site-representativity)

- EMEP defaults as given in Simpson et al. (ACP, 2012)
  - Inert POA
  - Derived from official PM2.5, plus assumed split into OM, EC, other-
    PPM2.5 from IIASA
  - Avoids MSC-W making assumptions on ’missing’ emissions
  - VBS for remaining OA
- Uses for annual reports, S-R matrices, etc.
POA: what does EMEP do now?  2. The Research Approach

  - volatile POA
  - Added SVOC/IVOC
  - POA-associated S/IVOC = 1.5 x POA-inventory
  - OM emissions from research projects, e.g. EUCAARI, TNO
  - Scientifically more realistic in principle – BUT – assumptions are very uncertain!

- See also Simpson & Denier van der Gon, EMEP Report 1/2015 (fig.)
SOA : SVOC+IVOC emissions 'assumed'

- Shrivastava et al. SVOC + IVOC = 1.5 x PM.
- ... not default in EMEP, tested in Bergström et al. 2012
Inert POA vs volatile/VBS POA

- Example given in Simpson et al. (ACP, 2012)
- Compared `policy` inert approach with `PAA` research approach of Bergström et al. (ACP, 2012)
- Relative fractions (left) show that inert assumption gives e.g. higher OM over Paris, but lower in many other areas (due to aging of SVOC/IVOC)
Modelling results (Bergström et al., 2012)

The **Good**

The **Bad**

The **Ugly**

TC$_{10}$ summer

TC$_{10}$ winter

Measured

Wood burning OC winter

Again: problem with inventory?
New emission inventory for residential biomass combustion (Denier van der Gon et al., 2015, Genberg et al, 2013)

- Emissions treated in a consistent way
- Emission factors based on dilution tunnel measurements
- Higher organic aerosol emissions than earlier inventories
- See talk by Jeroen Kuenen et al.
EMEP OA: not 'ok' in winter - likely due to emissions.

Fig from Denier van der Gon, ACP, 2015

See also Genberg et al, ACP, 2013, Simpson et al., JGR, 2007

And Jeroen’s talk!
Emerging issues? Diesel IVOC

Dummore et al. (ACP, 2015) found major underpredictions in long-chain HC in London air, ca. factor 4 for C9, factor 70 for C12!

These were estimated to have major impact on OH, O3

Ots et al., 2016 (ACPD, 2016) used these data to estimate IVOC (fig. above), in proportion to VOC (not PM2.5) emissions....
Diesel IVOC cont., Ots et al (EMEP4UK) results

**EMEP4UK setup**

**5x5 km2 resolution**

**Inert POA + VBS for SVOC,IVOC**
OA: Status and future ..... 

- (S)OA schemes keep changing
  - Fixed yields
  - G/P partitioning
  - Polymers
  - Oligomers
  - Sesquiterpenes
  - Aging
  - Emissions
  - Non-equilibrium

- And when the models give too much OA, we can add:
  - Fragmentation
  - Photolysis
  - More deposition
  - etc.

- Conclusion: model vs observed 'scatterplots' are a poor indication of true model performance. Need to check inputs independently!
POA: Conclusions

- Emissions:
  - The basic emissions factors (EFs) are likely the main source of errors
  - But volatility complexities can have major impact on these EFs
  - .. and S/IVOC assumptions can have major impact on SOA
  - Large need for new measurements, in ‘realistic’ conditions
  - These should account for volatility, S/IVOC, etc, as far as practical.
  - We need to know what we have in the inventories!