Local Fractions for O3 chemistry and source allocation

Peter Wind, EMEP/MSC-W
The Local Fraction method

- Originally developed to give the fractions of pollutants from local sources. Used for downscaling (uEMEP)

- A technical method to track a large number (10 000 s) of pollutant sources.
The Local Fraction for non linear species

- New: can track pollutants through chemical reactions

- Must track all pollutants involved in the reactions
  - only a few hundred sources can be tracked

- Gives the **sensibility** to (small) changes in emissions

Sensibility: \( S_{i,k}^{\text{NOx}} = \frac{\partial C_i}{\partial E_{k,\text{NOx}}} \quad S_{i,k}^{\text{VOC}} = \frac{\partial C_i}{\partial E_{k,\text{VOC}}} \)

For example \( \frac{\partial \text{O}_3}{\partial E_{k,\text{NOx}}} \), how much Ozone changes for changes in NOx emissions in region k.
Adjoint or sensitivity principle

Chemistry module (non linear)

Compute Jacobian \( \frac{\partial C_i(t+\Delta t)}{\partial C_j(t)} \)

Sensitivity updates:

\[ S^k_i (t+\Delta t) = \sum_j S^k_j (t) \cdot \frac{\partial C_i}{\partial C_j} \]

k: emission source
i,j: species
Source attribution

- Sensibilities only give effect of small emission changes.
- Linear only for small changes
- Sensibilities can be computed for many emission levels
- Use the complete species/emissions relationship to attribute pollutants to sources
Path Integral Method (A.M. Dunker 2014)

• Integrate sensibilities along a path between two emission scenarios

• For example
  scenario1: no anthropogenic emissions,
  scenario2: full emissions

• Gives a linear picture of contributions from regions
NL O₃ concentrations, July
All anthropogenic VOC NOx emissions 0->full
NL $O_3$ concentrations, February
All anthropogenic VOC NOx emis 0->full

![Graph showing the relationship between O3 change [ug/m3] and anthropogenic emissions [relative]. The graph includes lines for different categories such as O3, sum deltas, etc., indicating a linear decrease in O3 change as emissions increase.]
Summary

• Local Fractions allow to compute the concentrations/emissions relationship over a large emission range.

• How to use and present all this information?
The End
All species involved in O3 chemistry (54) must be tracked separately

Computational cost of a single run * 10

Non-linear
Computational cost (Chemistry part)

- $N_{\text{chem}}$: number of Chemical species (111 -> 54)
- $T_{\text{chem}}$: time to run «normal» emep Chemistry
- $N_{\text{countries}}$: Number of countries to treat ($51 \cdot 2$)
- $t$: very small time

- Cost(\text{BruteForce}) = N_{\text{countries}} \cdot T_{\text{chem}}$
- Cost(\text{LF})= N_{\text{chem}} \cdot T_{\text{chem}} + N_{\text{countries}} \cdot N_{\text{chem}} \cdot t$

- In practice: 9-12 times cost of single run
  (16 hours @24 nodes EMEP0302 for 1 year)