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State of (S)OA: an EMEP modelling perspective

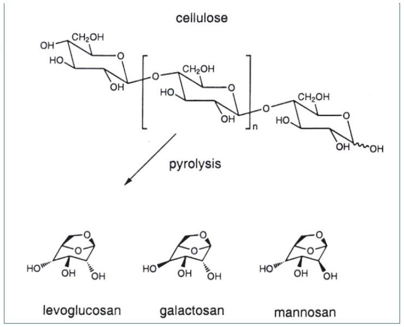
David Simpson

08/05/19

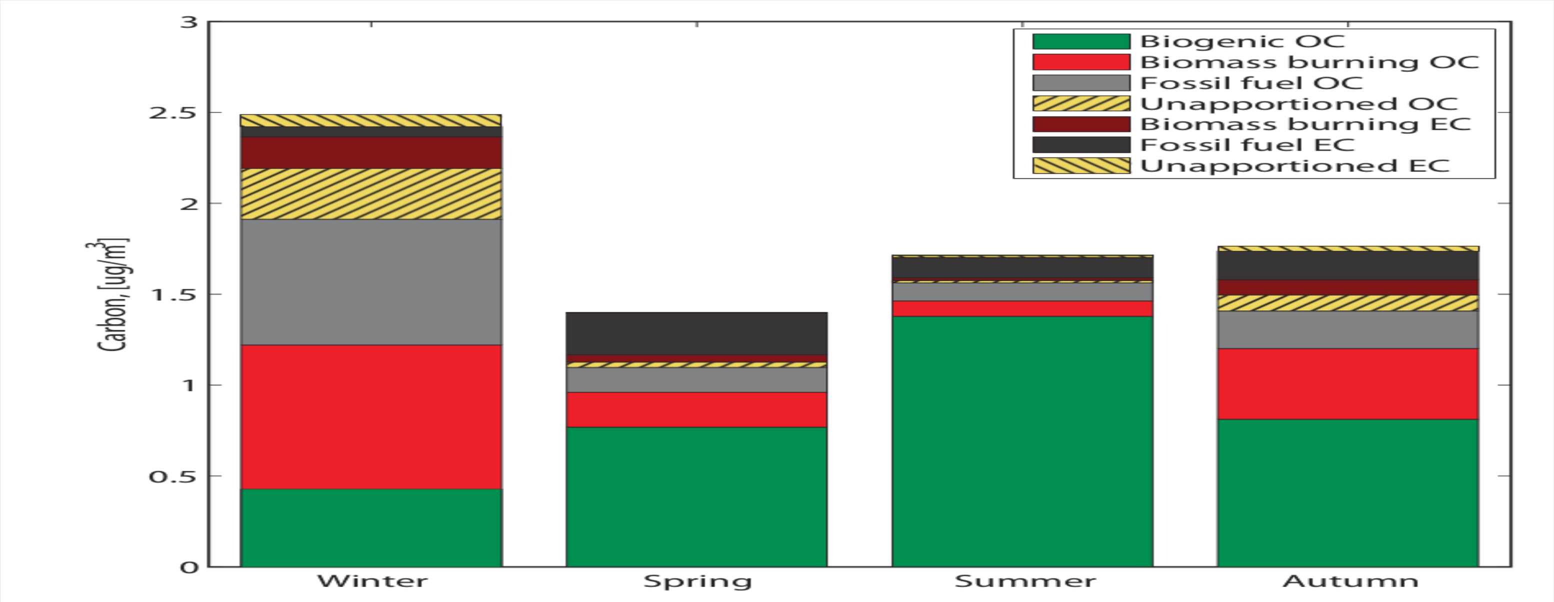
OA: what do we know?

- Source-apportionment – can be done with:
  - Tracers (e.g. levoglucosan or 14C) – eg Szidat et al., Yttri et al., Genberg et al., Glasius et al., ...
  - PMF of AMS data e.g. Lanz et al., Crippa et al., Mohr et al.,

- Levoglucosan tracer for biomass burning



Genberg et al 2011



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Summary of S-A

Source-apportionment in Europe shows:

- Summer OM dominated by BSOA
- Winter OM dominated by biomass-burning
- PBAP an issue for PM10
- Spring and Autumn are mixtures of above

This is both good (simple!)

Summary of S-A

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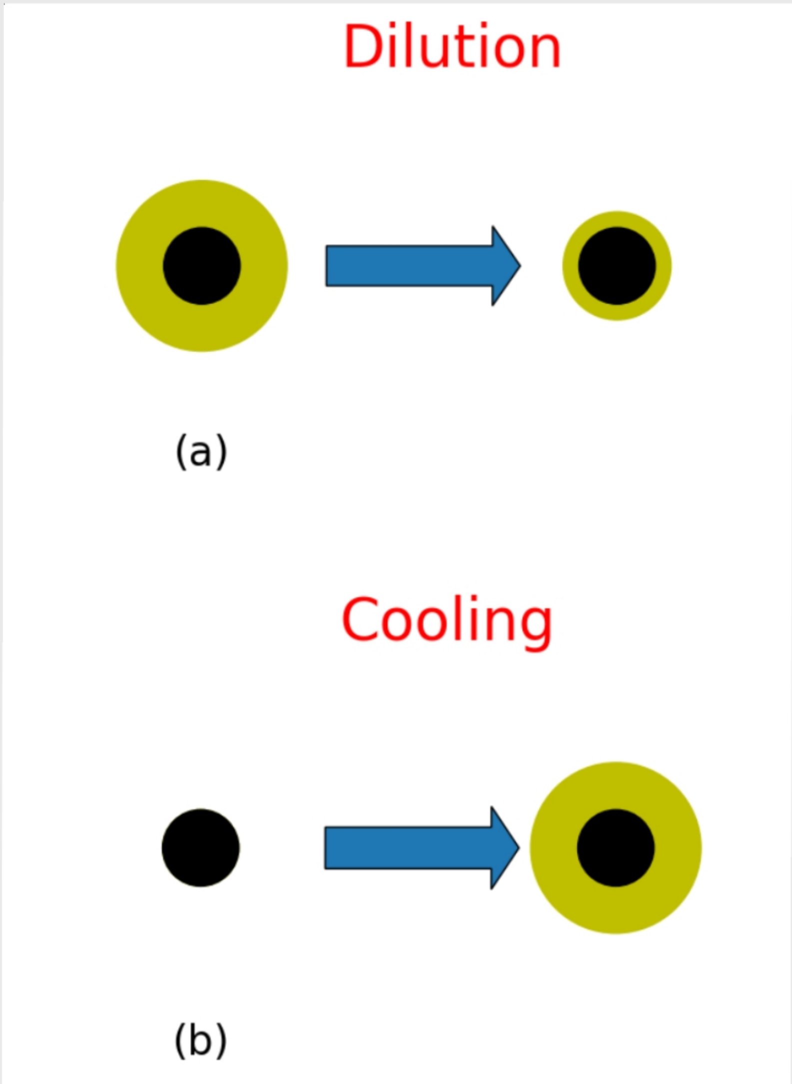
This is both good (simple!)

and bad!

- These are the hardest emission sources to pin down

OA emissions

- Problems of OA emissions by now well known...
- SVOC – IVOC - condensables
- See e.g. Denier van der Gon et al., ACP, 2015, Simpson and Denier van der Gon, EMEP 2015, Ots et al., ACP, 2016
- TFEIP-TFMM Proposal....
- Basically, countries report apples and oranges!



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Modelling of condensables

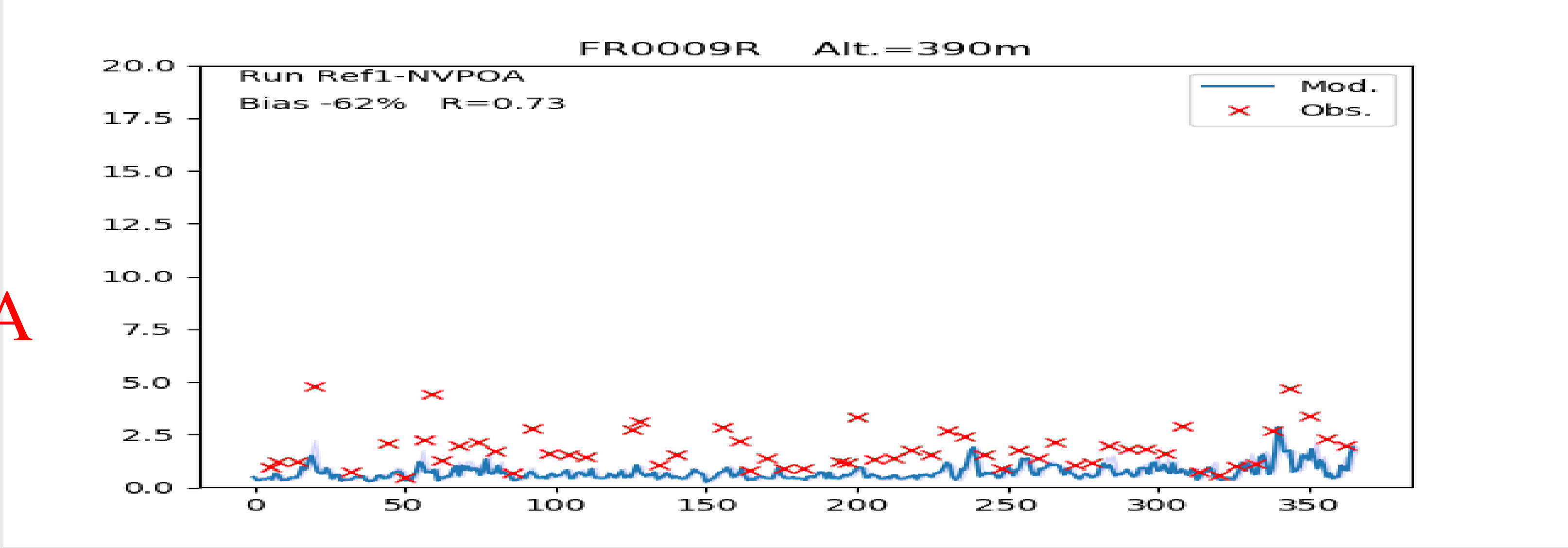
(with Robert Bergström, Hugo Denier van der Gon & TNO colleagues)

- Tested 4 cases:
  - a) Ref1, Inert POA. Emissions of POA as given in inventory. (NVPOA)
  - b) Ref1, treat as semi-volatile POA. (SVPOA)
  - c) Ref2 with TNO estimate of condensables, treated as non-volatile (NVPOA)
  - d) Ref2, treat as semi-volatile (SVPOA)

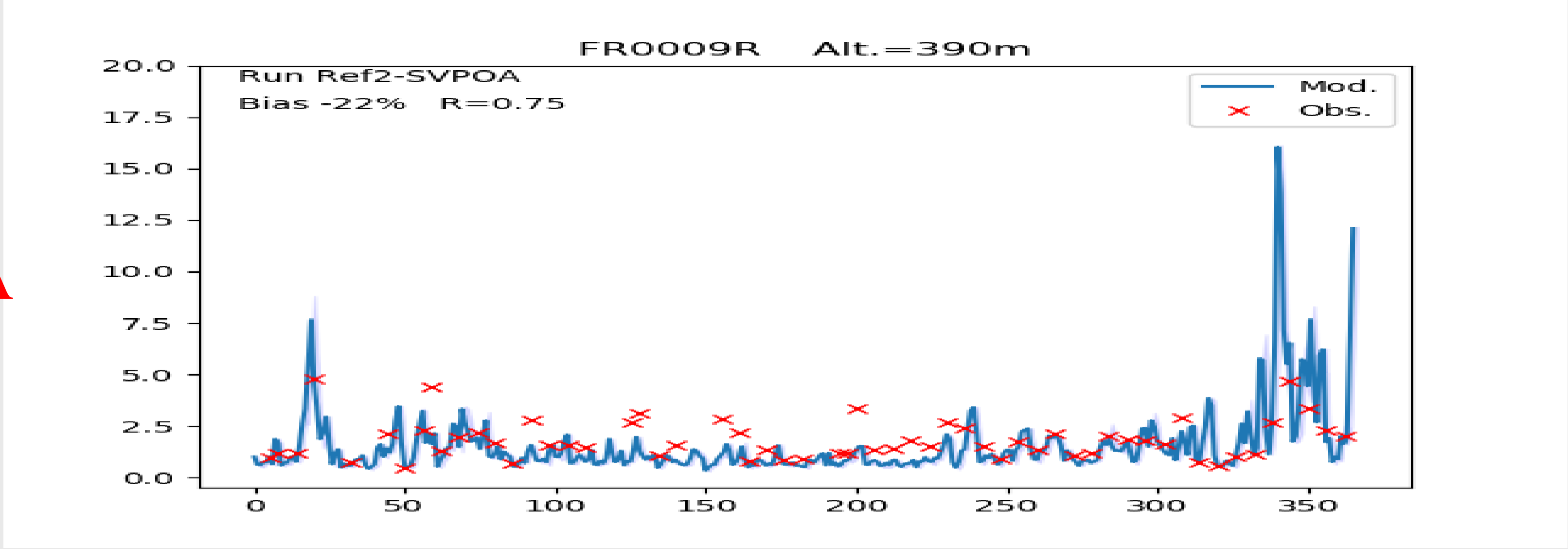
- All VERY uncertain!

Modelling of condensables, France (FR09)

Ref1-
NVPOA

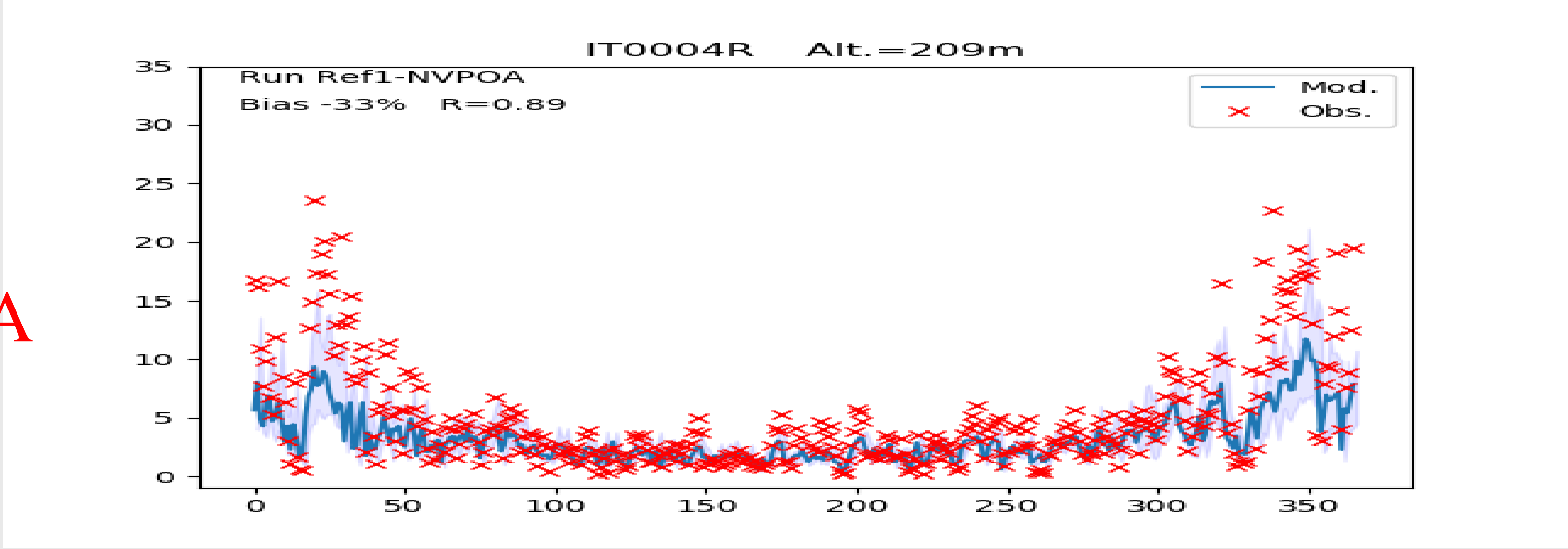


Ref2-
SVPOA

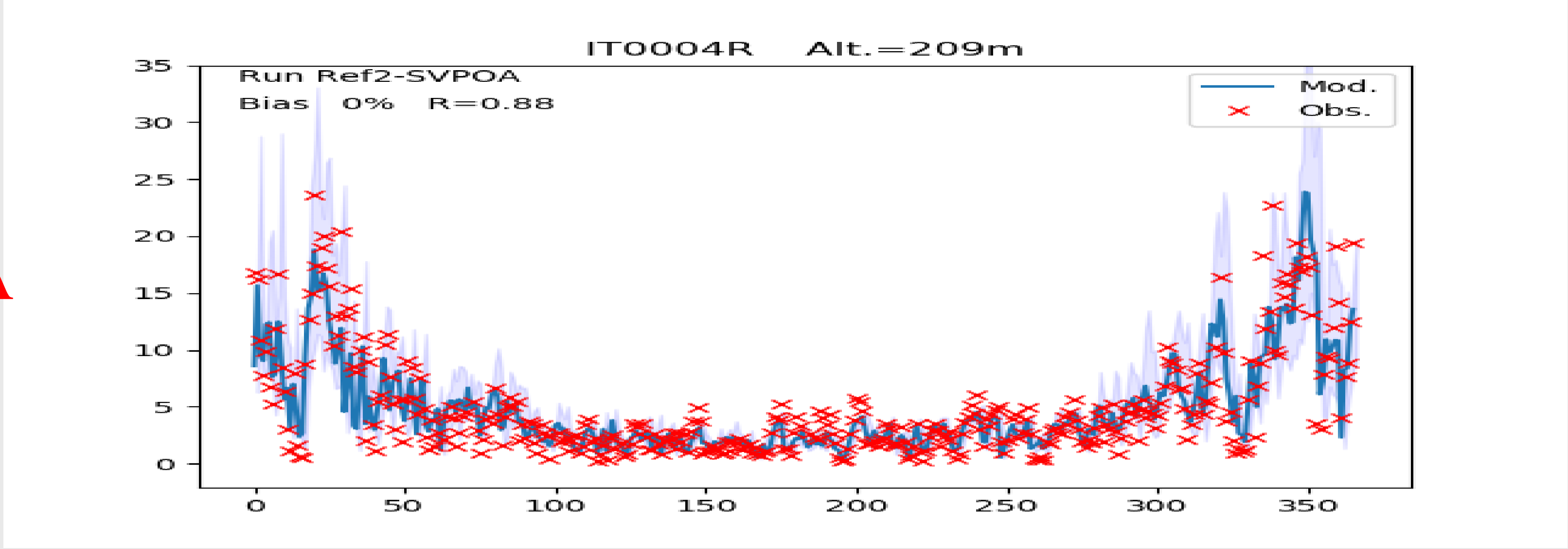


Modelling of condensables, Italy (IT04)

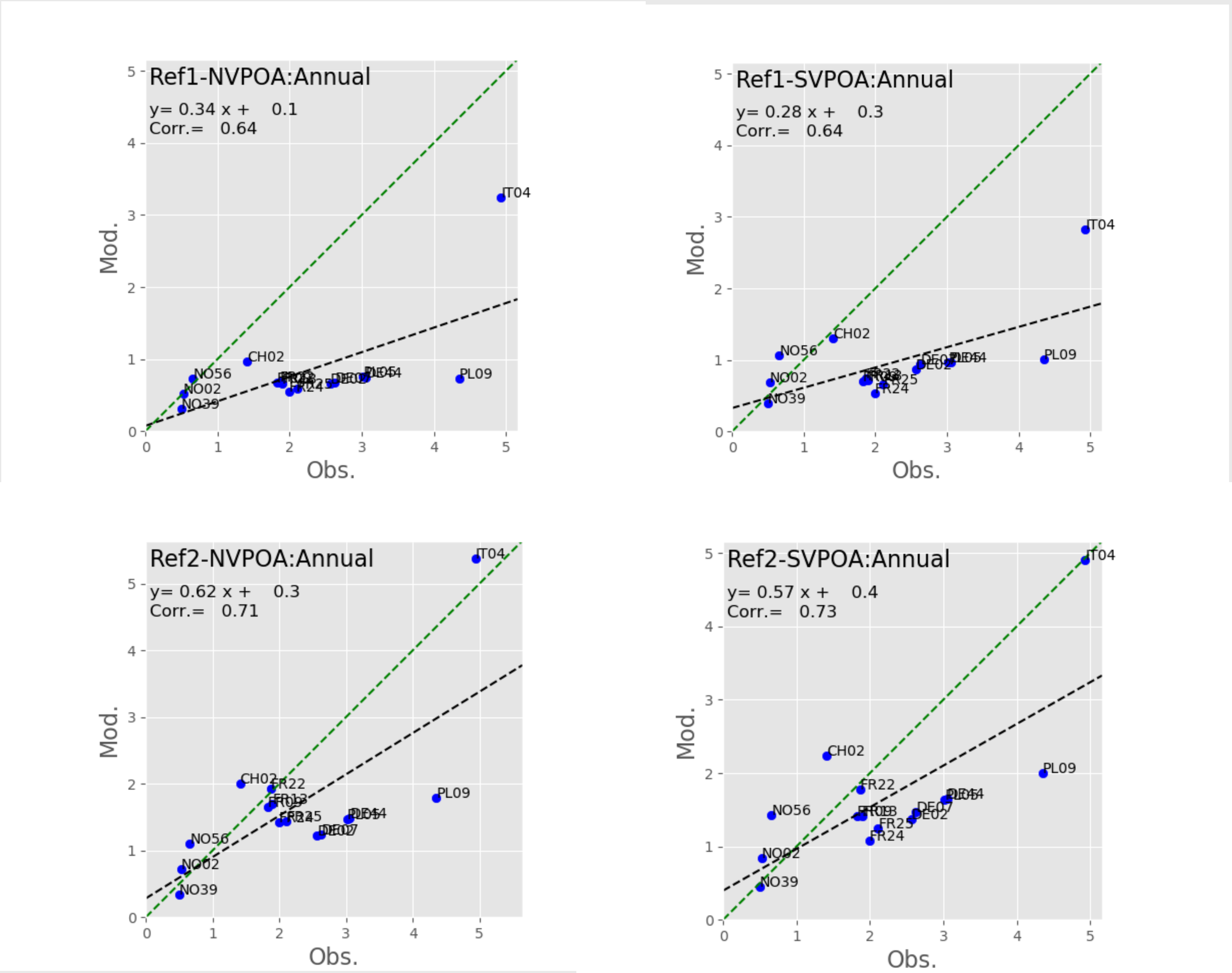
Ref1-
NVPOA



Ref2-
SVPOA



Modelling of condensables, cont.



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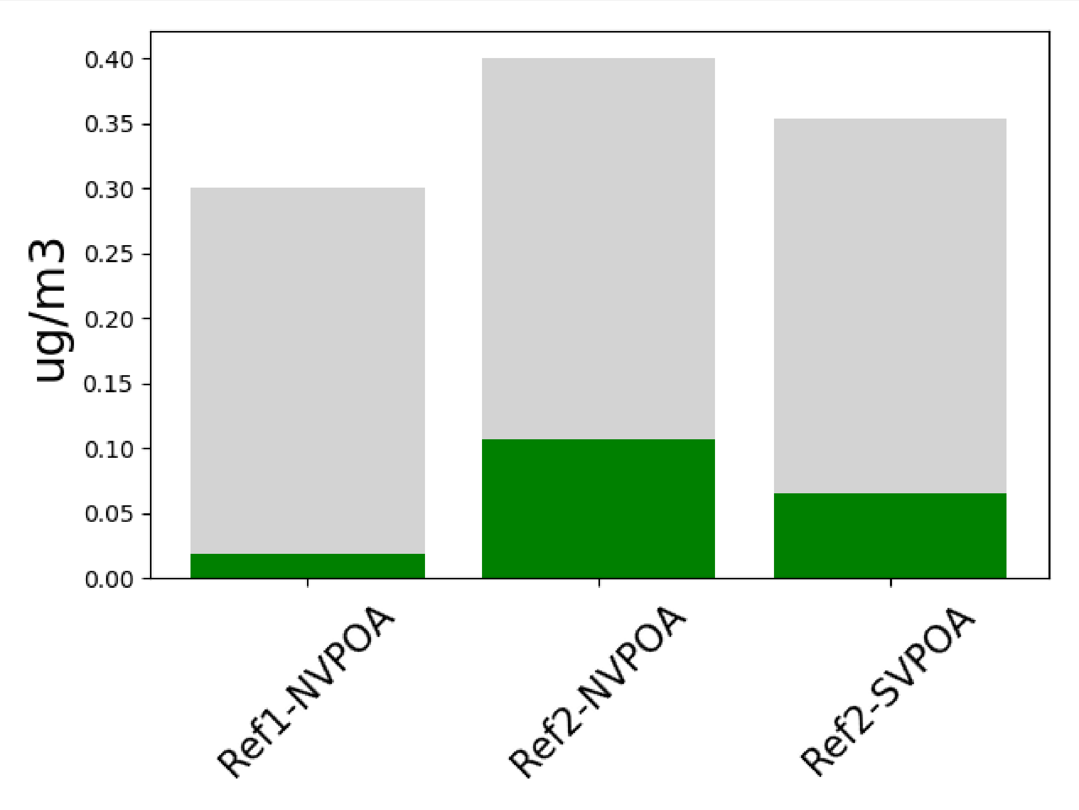
Condensables, impact on S-R matrices



Impact of 15% Netherlands emission reductions to $PM_{2.5}$ in own country, with runs Ref1-NVPOA, Ref2-NVPOA and Ref2-SVPOA

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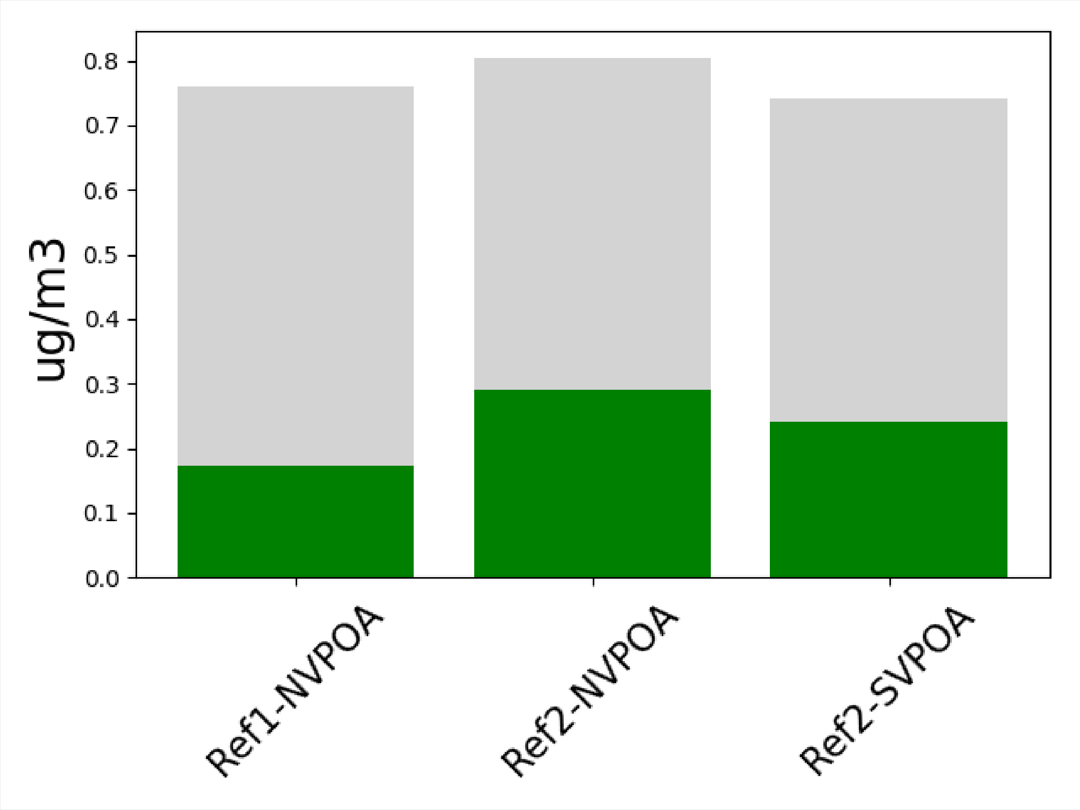
Condensables, impact on S-R matrices



Impact of 15% Italian emission reductions to $PM_{2.5}$ in own country, with runs Ref1-NVPOA, Ref2-NVPOA and Ref2-SVPOA

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Condensables? The TFEIP-TFMM note

- TFMM note tries to define which sectors include condensables, which don't.
- Country information is starting to come in (13 countries)
- Very complex information
- Apples and oranges within each country, and between countries
- Another consequence: if e.g GAINS suggests x% reduction in $PPM_{2.5}$ emissions, which PM does it assume ?!
- 2 year time-scale?! Gulp!

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POA/SVOC/IVOC: Conclusions

- The basic emissions factors (EFs) are likely the main source of errors in modelling POA and some SOA
  - and S/IVOC assumptions can have major impact on SOA
  - Large need for new measurements, in ’realistic’ conditions -- these should account for volatilty, S/IVOC, etc, as far as practical.
- In shorter term
  - PM inventories need to be harmonised
  - we need to know what we have!! (Apples or organges?)
  - Emissions (eg IVOC) are changing very quickly
  - Should the ’modellers’ be allowed to add these?
  - See & discuss TFEIP-TFMM Note

Back to modelling: EMEP SOA schemes in testing:

- 1-5D VBS (Koo et al. AE, 2014)
  - Some scientific advantages over VBS
  - New data/parameters from European RWC (Ciarelli et al., GMD, 2017)
- 'Hodzic' scheme – faster production, faster loss (Hodzic et al., ACP, 2016)
  - Pro:
    - Simpler yield definitions
    - Avoids 'zombie' SOA formation
  - Cons:
    - Too fast production close to source
    - Yields based upon OH reactions
- 'JPAC' models - based on plant-chamber yields
- 'ESM' - testiing Earth System Model schemes (e.g. EC-Earth, NorESM)

- All schemes make many arbitrary assumptions, concerning e.g. deposition rates, emissions, SVOC, etc.

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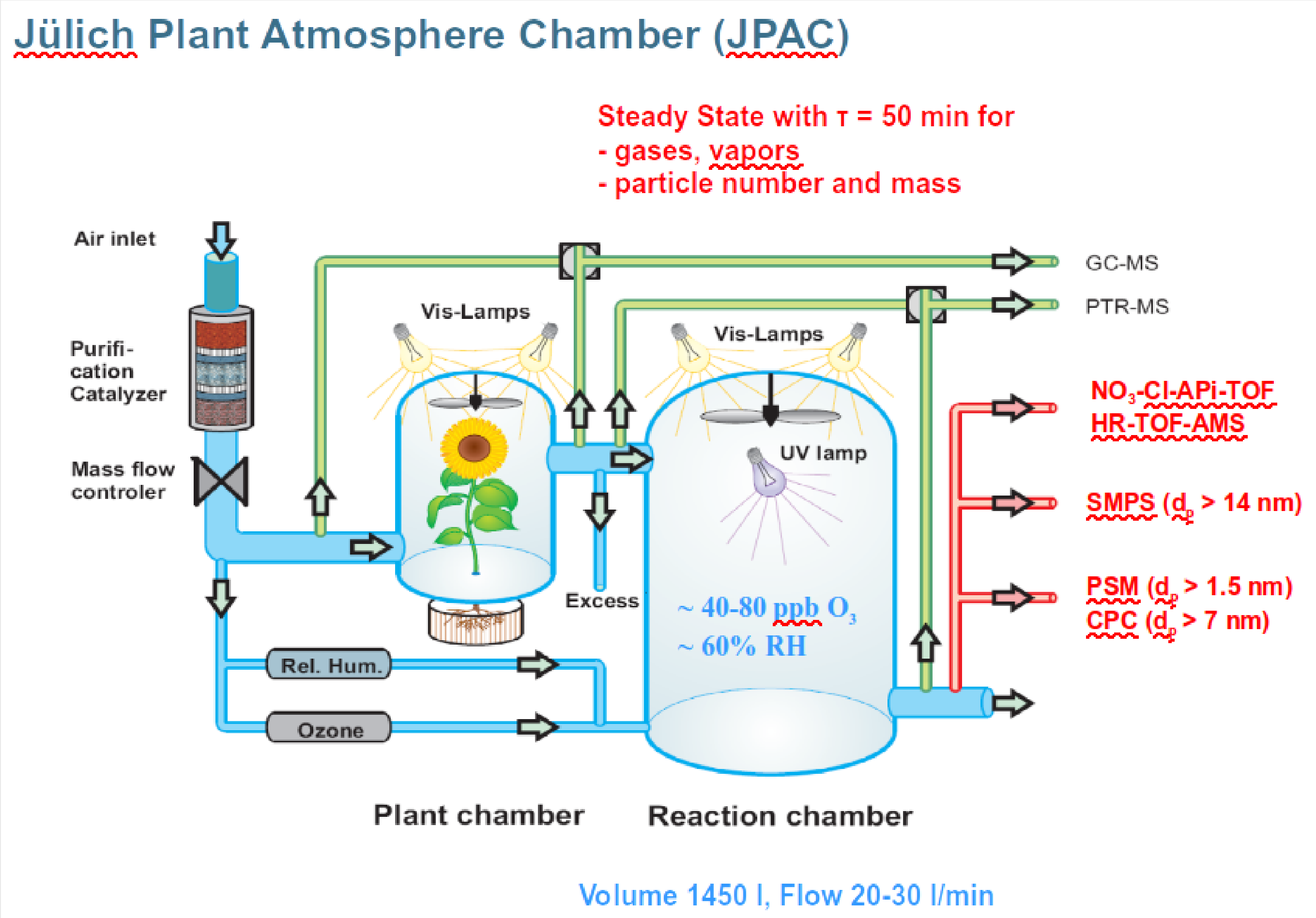
Example: modelling OC – from plant to atmosphere.....

Cooperation between Gordon McFiggans, Mattias Hallquist, Thomas Mentel, David Simpson et al



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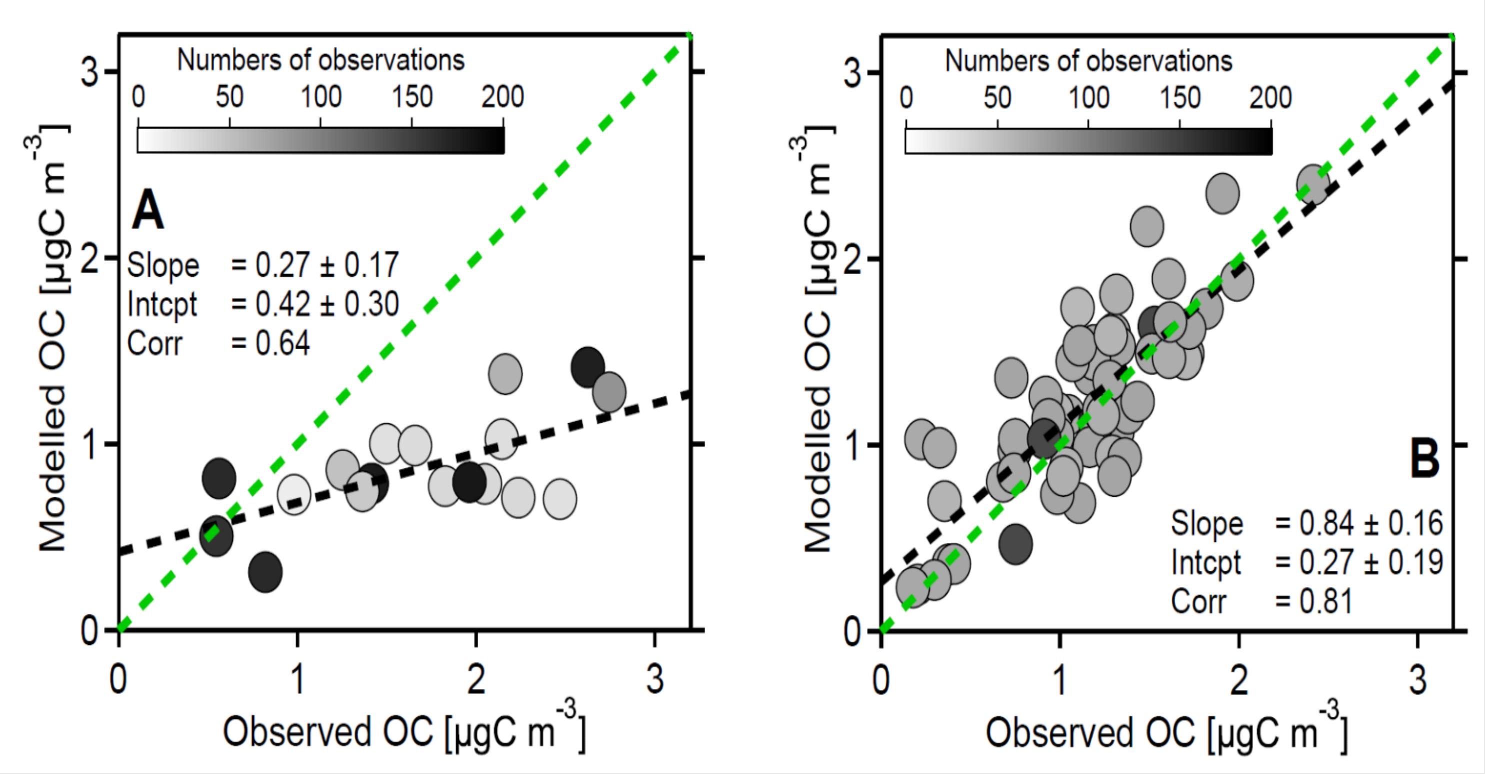
even simple schemes can work.....

- EMEP model + BSOA yields derived from JPAC chamber
- Compare OC with European (left) and American (right) OC



McFiggans et al, Nature, 2019

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Example 2 – evaluation of EC-Earth schemes in EMEP model

Robert Bergström (+ thanks to Pontus Roldin)

- Background:
  - EC-Earth has very simple SOA schemes
  - Evaluation limited
- Approach
  - Run EMEP model with several SOA schemes, incl. 2 from EC-Earth (also using new emissions inventory from TNO)
  - Compare
- CAVEAT
  - Just started! Scheme needs checking....

AVOC-SOA (O'Donnell et al., 2011; mass-based yields, from Ng et al., 2007, low NOx conditions)

Benzene + OH → 37% SOA
Toluene + OH → 36% SOA
Xylenes + OH → 30% SOA

Monoterpenes + OH → 25.7% BSOA
Monoterpenes + O_3 → 26.2% BSOA

Isoprene + OH → 3.4% BSOA
Isoprene + O_3 → 3.4% BSOA

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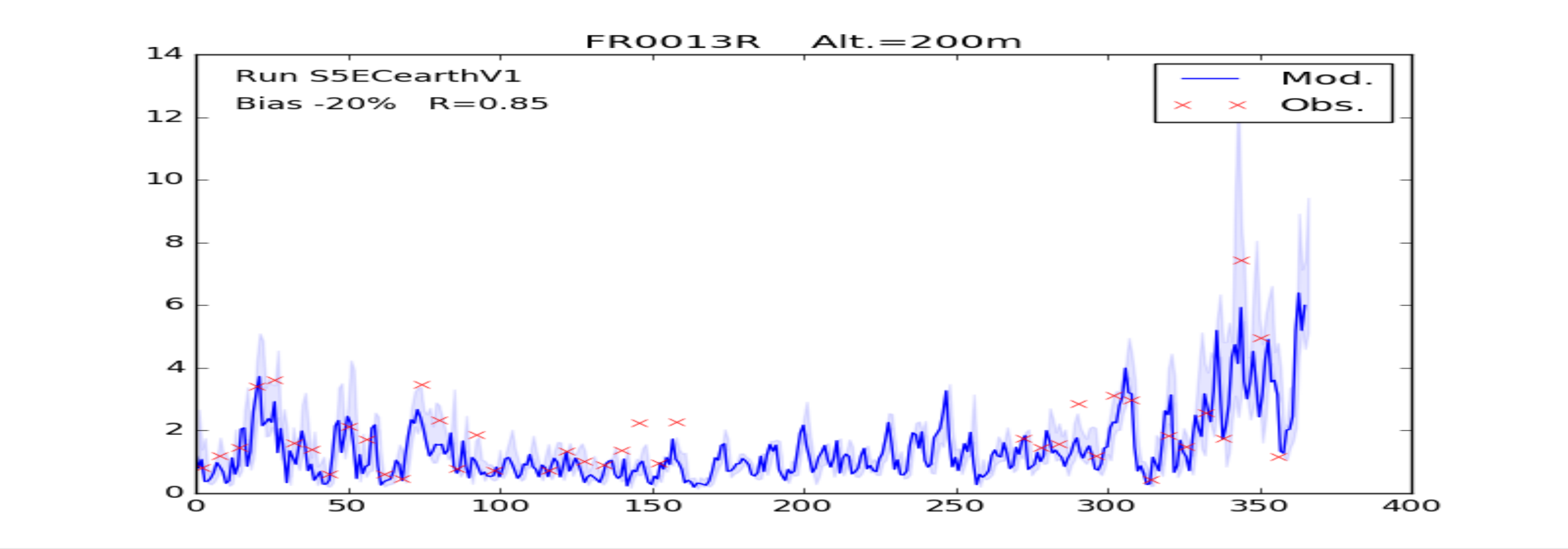
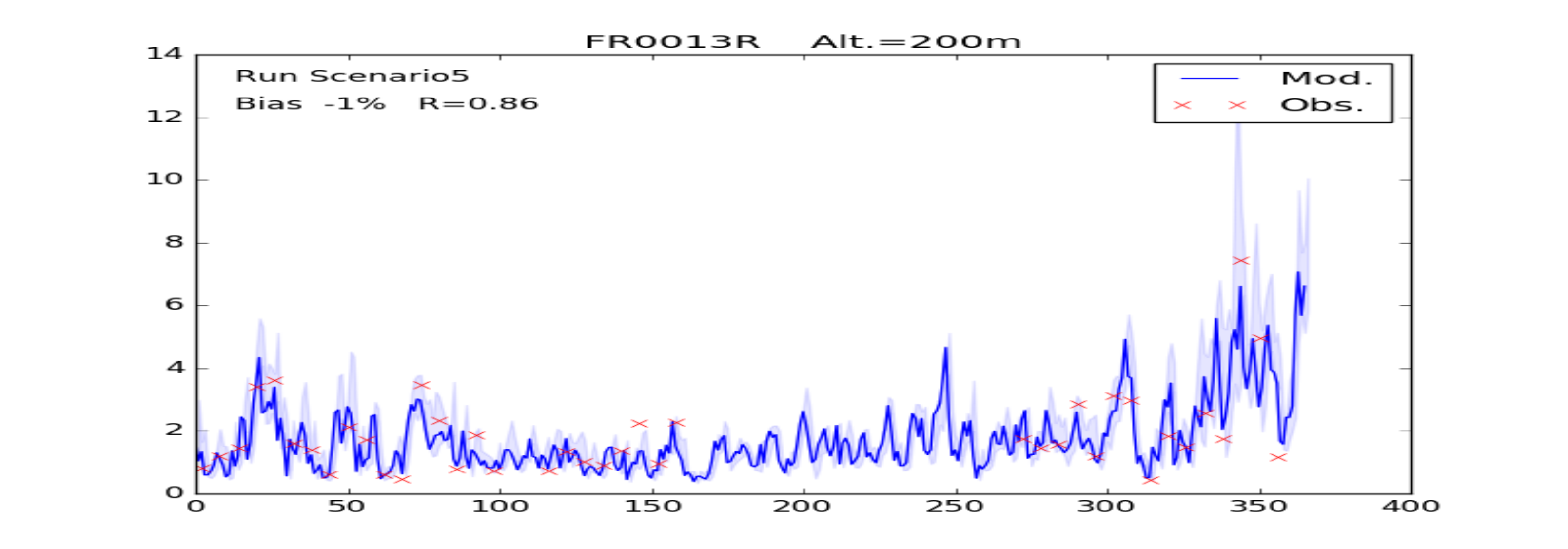
OC, France, EC-Earth v1 & EMEP, 2016

EC-Earth

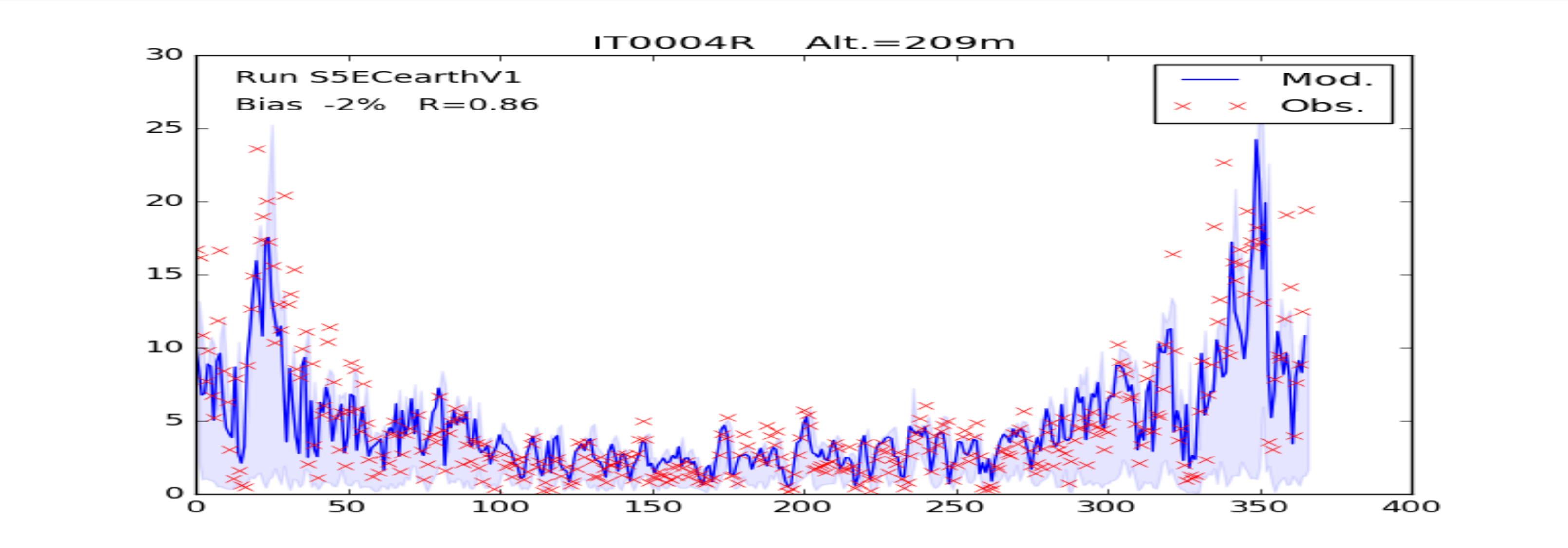


EMEP



OC, Italy, EC-Earth v1 & EMEP, 2016

EC-Earth



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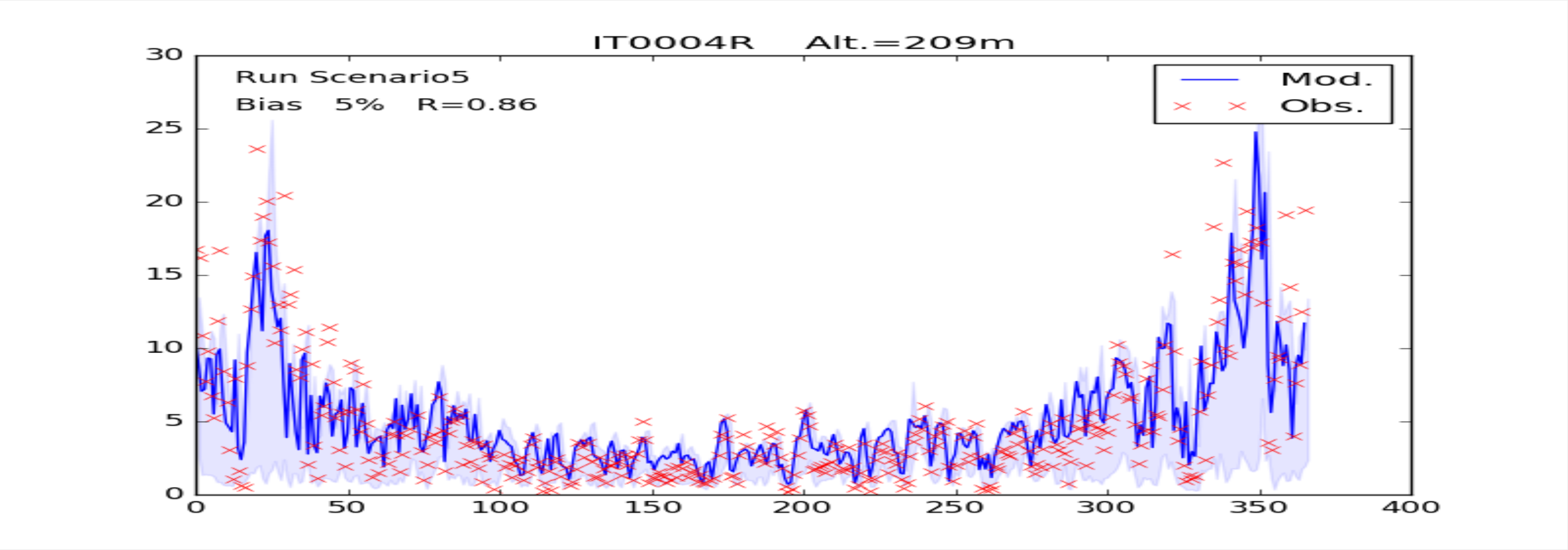
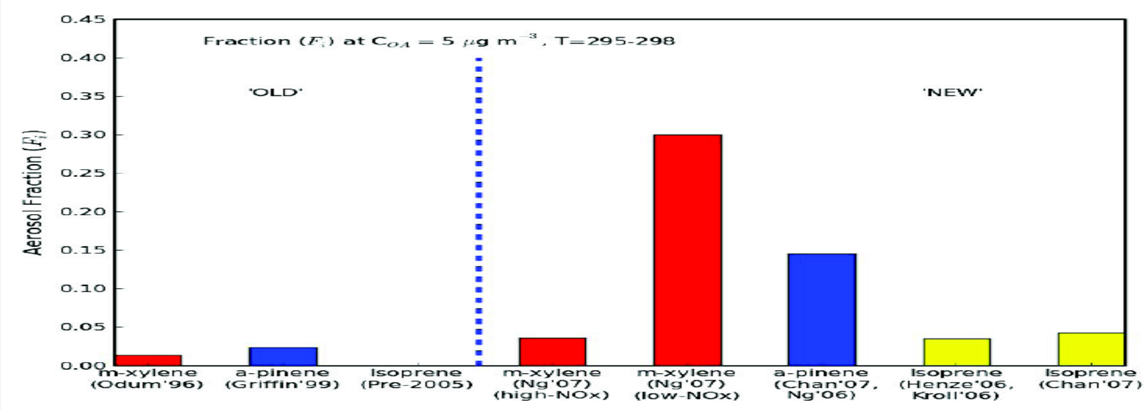


Evaluation of EC-Earth schemes in EMEP model: Conclusions?



(Fig Hallquist et al, ACP, 2009)

- Very preliminary!!
  - (Results are 'hot off the press')

  First results very promising!
  - Compares almost as well as EMEP schemes with European data
  - Not well evaluated at fine-scale
- Caveat
  - Some of the assumptions behind the scheme are VERY questionable, e.g. that all aromatics are in 'low-NOx' environments.
  - This would affect S-R results!

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(S)OA: Conclusions

- The basic emissions factors (EFs) are likely the main source of errors
- But volatility complexities can have major impact on these EFs
- S/IVOC assumptions can have major impact on modelled OA
- Issues are VERY complex
- We need to know what we have in the inventories!
- OA models can do well .... for many wrong reasons!
- Large need to constrain OA models with observations!