Assignment 4: Extended Outline

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1 Introduction

Currently Accepted General Statement

- VOCs have an adverse effect on health, both directly and indirectly as a precursor of secondary air pollutants, such as O3. [Laurent:2014]
- Degradation of VOC in the presence of NOx and sunlights leads to increased levels of tropospheric O3 [Atkinson:2000].
- Chemical transport models are numerical models that used to predict air pollutant concentrations (such as O3 or PM) for different emission scenarios ⇒ representing VOC emissions in models is critical.
- Emission Inventories (EIs) split VOC emissions into sectors according to their source (e.g. Industry, Solvent Use). Sectors are further split into VOC groups and/or individual VOC with relative contributions to total sector emissions.

Specific Problem(s)

- Uncertainties in EI: are the VOC and their contributions correct? [Borbon:2013]
- EI are static i.e. represent a snapshot in time whereas VOC emissions from a sector are not constant in time. [Boynard:2014]

Gap

- Need for more (spatial and temporal) representative and accurate EIs.

Study Objective/Scientific Question/Hypothesis

- Would changing an EI make a difference to modelled output? Focus on O3 produced from different solvent sector EIs, as solvent sector has largest contribution to total anthropogenic emissions.

2 Materials and Methods

2.1 Solvent Sector NMVOC Speciations

- Reference: TNO (European average) compared to model (IPCC, EMEP) and country (DE94, GR95, GR05, UK98, UK08) speciations. Table: Initial Speciation VOC assigned to categories
- Solvent speciations determine the model inputs i.e. which VOC and how much is emitted.

2.2 Model Description

- Boxmodel to focus on impacts of VOC emissions on O3 production chemistry.
- Use MECCA boxmodel similarly set up as described in [Coates:2015].
- MCM v3.2 chemistry: $\sim$120 primary VOC with detailed degradation chemistry.
- Does changing the chemistry scheme reduce or enhance the O3 produced from the EIs? Use regional and global chemistry schemes (RADM2 and MOZART) with same model setup.

- Used MOZART and RADM2 as described in [Coates:2015].

2.3 Model Set-up and Simulations

- Conditions for maximum O3 production for each speciation.

- 7 day run time as not all VOC produce maximum O3 on the first day.

- Idealised urban area of 1000 km^2, total NMVOC emissions of 1000 tons day^{-1}.

2.4 NMVOC Initial Conditions

- Solvent sector contributes 43% to total NMVOC emissions $\Rightarrow$ Total NMVOC emissions in each run = 430 tons day^{-1}

- Emitted VOC and amount emitted determined from different speciations, if a VOC group is specified, the individual VOC are determined using [Passant:2002].

- NMVOC emissions held constant until noon of first day.

- Table: MCM initial conditions for each speciation.

3 Results

3.1 Ozone Time series

- Figure: [O3] time series.

- Model speciations give highest O3 for all mechanisms.

- MCM: 17 ppbv between highest and lowest time series. Speciation profiles are relatively evenly spread out time series but EMEP higher.
- MOZART: 12 ppbv between highest and lowest time series. Time series have less spread but IPCC much higher on first 2 days.
- RADM2: 17 ppbv between highest and lowest time series. IPCC and EMEP outliers compared to other speciations.

3.2 Ox Production Budgets

- Figure: Ox production budgets allocated to original categories, using tagging technique.
- Same relationships of O3 time series also seen.
- Alkanes and oxygenated VOC dominate Ox production.

3.3 Alkanes and Ox Production

- Figures: Correlations of Alkanes and Oxygenated VOC in EI vs Ox production.
- More alkanes $\Rightarrow$ more Ox, more oxygenated $\Rightarrow$ less Ox.

4 Discussion

4.1 Ozone Time series

- In our study, the choice of input VOC speciation and chemical mechanism in the model influences the simulative O3 mixing ratios.

- Li:2014 compared O3 produced from different EIs used for East-Asia, focusing on individual VOC and how the different contributions specified influences the O3 produced from the individual VOC.

4.2 Ox Production Budgets

- Alkanes have a larger potential to produce Ox over multi-day runs than more reactive VOC [Butler:2011, Coates:2015].

- MOZART underestimates Ox from aromatics and alkanes compared to MCM [Coates:2015] $\Rightarrow$ Ox production in MOZART $<$ MCM.

- RADM2 underestimates Ox from aromatics and many alkanes, Ox production from smaller alkanes over estimated compared to MCM [Coates:2015] $\Rightarrow$ speciation determines whether the Ox produced with RADM2 is greater or less than MCM.

4.3 Alkanes and Ox Production

- IPCC and EMEP with highest Ox production specify more alkane than oxygenated species from solvent sector, whereas all other speciations specify the opposite and have lower Ox production.

- Li:2014 analyse Ox production from individual VOC using the MIR scale $\Rightarrow$ underestimation of alkanes compared to reactive VOC. Thus they conclude that alkenes and other more reactive species have the largest impact on O3 production.

- Are alkanes represented correctly (type and contribution)?

- Improved estimates for VOCs and their contributions in EIs.

5 Conclusions

- Our modelling study suggests that the choice of VOC speciation influences O3 mixing ratios.
- Speciations allocating more emissions to alkanes produce more O3 than speciations with more contributions of oxygenated species under the conditions of the model.
- Going from a boxmodel to a 3-D model may reduce these differences in O3 due to effects of transport and dilution.