Meteorology and Ozone, Temperature

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Abstract

1 Introduction

2 Methodology

2.1 Model Setup

- MECCA box model as described in Coates and Butler (2015) to broadly simulate the benelux (Belgium, Netherlands and Luxembourg) region. Solar zenith angle of 51°N was used to determine photolysis rates through a parameterisation and the SZA chosen is broadly representative of the central benelux region.

- MECCA box model has been updated to include vertical mixing with the free troposphere and accordingly includes a diurnal cycle for the PBL height. These amendments are discussed further in Sect. 2.3.

- All simulations performed using the Master Chemical Mechanism, MCM v3.2, (Rickard et al., 2015) and also repeated using MOZART-4 (Emmons et al., 2010). Coates and Butler (2015) describes the implementation of both MCM v3.2 and MOZART-4 for use with KPP within MECCA.

- NOx and other parameters were varied systematically to analyse the effects on ozone mixing ratios over different NOx gradients and hence different atmospheric conditions.

- VOC emissions constant until noon of first day, to simulate a plume of emitted VOC.
- Simulations start at 06:00 using spring ecquinoctical conditions and the simulations ended after two days.

2.2 VOC Emissions

- Anthropogenic emissions from the Benelux regions were determined using the TNO-MACC_III emission inventory; the TNO-MACC_III inventory is the latest update of the TNO-MACC_II inventory and was created using the same methodology as (Kuenen et al., 2014) and based upon improvements to the existing emission inventory during the AQMEII 2 exercies described in Pouliot et al. (2015).
- Temperature independent emissions of the biogenic VOC isoprene and monoterpenes, were calculated as a fraction of the total anthropogenic VOC emissions from each country in the Benelux region, this data was obtained from the supplementary data available from the EMEP (European Monitoring and Evaluation Programme) model (Simpson et al., 2012).
- These emissions are included as total emissions from SNAP (Selected Nomenclature for Air Pollution) source categories and were assigned to chemical groupings based on the country specific profiles for Belgium, the Netherlands and Luxembourg provided in Builtjes et al. (2002). correct citation?
- The MCM v3.2 initial species were determined using the country specific profiles for each SNAP source category and where appropriate information of individual chemical species that can be represented by MCM v3.2 were determined using the speciations of Passant (2002).
- After calculating the MCM v3.2 initial VOC and respective emissions were assigned to the respective MOZART-4 species and the emissions in MOZART-4 were weighted by the carbon numbers of the MCM v3.2 species and the emitted MOZART-4 species.

2.3 Vertical Mixing with Diurnal Boundary Layer Height

- The base boxmodel (Sect. 2.1) includes a constant boundary layer height of 1 km and no interactions (mixing) with the free troposphere.

- A parameterisation of the diurnal profile of the planetary boundary layer (PBL) height over Los Angeles was provided by Boris Bonn based on data from the CARES field campaign (CARB, 2008) .

- The PBL height was calculated at every time point for the model run and then read into the boxmodel at each time point .

- The concentrations of the chemical species within the PBL are diluted due to the larger mixing volume when the PBL height increases at the beginning of the day, also the increasing PBL height induces mixing of chemical species from the free troposphere with those chemical species within the PBL i.e. vertical mixing. When the PBL height collapses during night giving the stable nocturnal boundary layer, this traps the chemical species into a smaller volume thus increasing the concentrations of the chemical species.

- This vertical mixing scheme was implemented into the boxmodel using the same approach of Lourens (2012).

- The mixing ratios of O3, CO and CH4 in the free troposphere were respectively set to 50 ppbv, 116 ppbv and 1.8 ppmv. These condions were taken from the MATCH-MPIC chemical weather forecast model on the 27th March (the start date of the simulations). The model results (`http://cwf.iass-potsdam.de/`) at the 700 hPa height were chosen and the daily average was used as input into the boxmodel.

- Tagged free troposphere species were also included in the boxmodel to determine effect of free troposphere species on surface ozone levels.

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3 Results

4 Conclusions

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