Meteorology and Ozone, Temperature, Relative Humidity

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Abstract

1 Introduction

Gap: Many observational studies have noted the dependence of ozone production on temperature and also the non-linearity of ozone production on temperature and NOx. Furthermore, many regional modelling studies have also reproduced this relationship of ozone production on temperature for specific areas; currently most of these modelling studies have been concerned with US regions. Despite all this research, there has not been (to our knowledge) a detailed process study looking at modelled ozone as a function of both NOx and temperature. In this study, we model ozone over various temperature and NOx levels to determine how ozone production varies under these range of conditions. The review of Pusede et al. (2015) also highlights a lack of modelling studies looking at this non-linear relationship of ozone on NOx and temperature.

Pusede et al. (2014) demonstrated the importance of tackling high ozone levels also from the stand point of temperature and in relation to varying NOx conditions over the San Joaquin Valley in California and the review of Pusede et al. (2015) highlights that the temperature dependence of biogenic VOC (BVOC) emissions is mainly responsible for this relationship. In this study, we model the effects of temperature-dependent and temperature-independent BVOC emissions on ozone production in order to look at the effects of temperature dependent ozone production chemistry without temperature dependent VOC emissions and then the effects of temperature-dependent chemistry and temperature-dependent BVOC emissions. As mentioned

in the review of Pusede et al. (2015), typically BVOC emissions are temperature-dependent while anthropogenic VOC (AVOC) emissions tend to be temperature-independent, as AVOC emissions tend to be process and combustion related.

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.

- Simulations start at 06:00 using spring equinoctical conditions and the simulations ended after two days.

- All simulations performed using the Master Chemical Mechanism, MCM v3.2, (Rickard et al., 2015), Common Representative Intermediates, CRI v2 (Jenkin et al., 2008), Model for Ozone and related chemical tracers, MOZART-4 (Emmons et al., 2010), Regional Acid Deposition Model, RADM2 (Stockwell et al., 1990) and the Carbon Bond Mechanism, CB05 (Yarwood et al., 2005). Coates and Butler (2015) describes the implementation of these chemical mechanisms for use with KPP within MECCA. These chemical mechanisms were chosen as they are commonly used by modelling groups and represent the highly-detailed chemistry (MCM v3.2), chemistry suitable for regional 3D models (CRI v2, RADM2 and CB05) and global 3D models (MOZART-4).

- NOx and emissions and temperature were varied systematically to analyse the effects on ozone mixing ratios over different NOx gradients and different temperatures.

- VOC emissions constant until noon of first day, to simulate a plume of emitted VOC.

- Two sets of runs were performed – to include both a temperature-dependent and temperature-independent source of biogenic VOC emissions. MEGANv2.1 (Guenther

et al., 2012) was used to specify the temperature-dependent BVOC emissions of isoprene. Isoprene is the most important VOC at a global scale due its high emission rates and emissions from vegetation have been reported to depend on temperature (Guenther et al., 2006).

- Methane is fixed at 1.7 ppmv throughout the model run, carbon monoxide (CO) and ozone were initialised at 200 ppbv and 40 ppbv and then allowed to evolve freely throughout the the simulation.

- The first set of model runs were performed using the MCM v3.2, the most detailed chemical mechanism used in the study. The NO emissions used in each model run were then used in when running the model at the same conditions (NOx and temperature) with all the other chemical mechanisms.

- NOx emissions are non-realistic and vary from XX to XX in each model run at the same temperature and each chemical mechanism.

Determine min and max NO from MCM runs

2.2 VOC Emissions

- Anthropogenic emissions from Benelux were obtained from the TNO-MACC_III emission inventory. TNO-MACC_III is the current version 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).

- AVOC and BVOC emissions are included as total emissions from SNAP (Selected Nomenclature for Air Pollution) source categories and these emissions were assigned to chemical groupings based on the country specific profiles for Belgium, the Netherlands and Luxembourg provided by TNO.

- The monthly relative emissions factors for the different SNAP categories were then used to determine the total NMVOC emissions for the month of March, as the model starting date

Table 1: Anthropogenic NMVOC emissions in March 2011 in tonnes from each SNAP category assigned from TNO-MACC_III emission inventory and biogenic VOC emission in tonnes from Benelux region assigned from EMEP. The allocation of these emissions to MCM v3.2, CRI v2, CB05, MOZART-4 and RADM2 species is found in the supplement.

	SNAP1	SNAP2	SNAP34	SNAP5	SNAP6	SNAP71
Belgium	4279	16912	23768	5454	45720	6539
Netherlands	9680	24285	28710	8731	52571	15942
Luxembourg	115	82	207	1373	4442	1638
Total	14074	41279	52685	15564	102733	24119
	SNAP72	SNAP73	SNAP74	SNAP8	SNAP9	BVOC
Belgium	2426	143	209	6494	821	7894
Netherlands	3104	1233	1723	9886	521	1564
Luxembourg	989	6	305	637	0	2155
Total	6519	1382	2237	17017	1342	11613

in March 21st. These monthly relative emissions factors were taken from EMEP data . reference

- 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 detailed speciations of Passant (2002).

- First the primary VOC that are represented by the MCM v3.2 and respective emissions were determind. Using this MCM v3.2 data, the NMVOC emission data were mapped to mechanism species in the other four chemical mechanisms used in the study. The NMVOC emissions in the non-MCM v3.2 chemical mechanisms were weighted by the carbon numbers of the MCM v3.2 species and the emitted mechanism species. The supplementary data outlines the primary NMVOC and calculated emissions with each chemical mechanism.

2.3 Vertical Mixing with Diurnal Boundary Layer Height

- The MECCA box model used in Coates and Butler (2015) includes a constant boundary layer height of 1 km and no interactions (mixing) with the free troposphere.

- The planetary boundary layer (PBL) height varies diurnally and affects chemistry by diluting emissions after sunrise when the PBL rises. The expansion of the PBL into the free troposphere introduces vertical mixing with those chemical species present in the free troposphere. When the PBL collapses in the evening, pollutants are trapped in the PBL.

- Boris Bonn provided a parameterisation of the diurnal profile of the PBL height based on data from the CARES field campaign (CARB, 2008) . This parameterisation was then used to calculate the PBL height at every time point for the model run and then read into the boxmodel at each time point. Figure 1 illustrates the diurnal profile used in this study.

  `check if reference correctly`

- 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 O_3, CO and CH_4 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 21st 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.

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Figure 1: The planetary boundary layer (PBL) height diurnal profile used in the study.
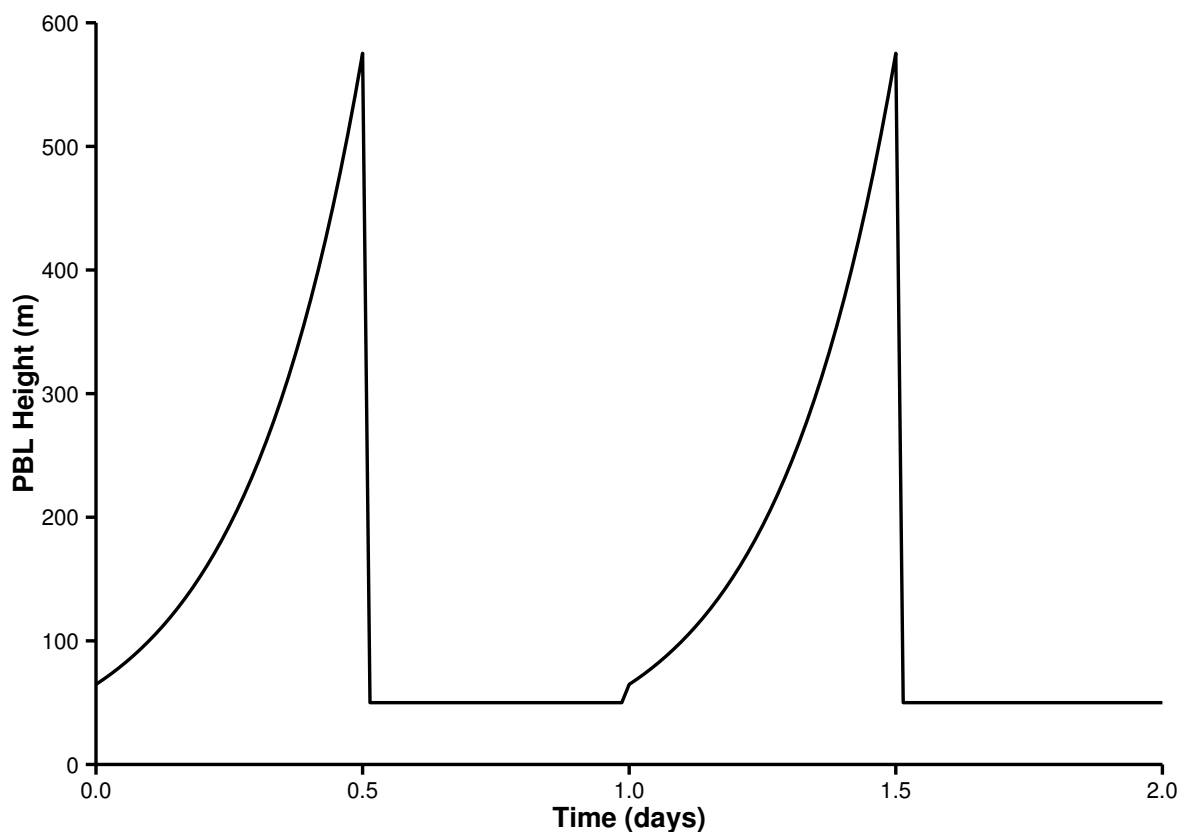
3 Results

4 Conclusions

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