

Modelling multiphase night-time processes with WRF-Chem

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Aerosol particles play an integral part in the chemistry of the atmosphere — by acting as reaction surfaces for heterogeneous chemistry, as chemical sources, and by removing components through scavenging and dry deposition. They have an important influence on the lifetime of the nitrate radical (NO₃), which is the dominant oxidant in the nocturnal atmosphere. NO₃ and NO₂ are in thermal equilibrium with N₂O₅, which acts as a reservoir species for NO₃. However N₂O₅ also provides an important loss pathway for NO_x by conversion to HNO₃ via heterogeneous reactions on aerosol particles, the rates of which are dependent on aerosol composition, relative humidity and temperature (Allan et al., 1999, Davis et al., 2008; Bertram & Thornton, 2009). In order to properly predict the oxidative capacity of the nocturnal atmosphere we must understand the influence of aerosols on gas-phase chemistry.

This study uses the WRF-Chem regional atmospheric chemistry model (Grell et al., 2005; Fast et al., 2006), with the MOSAIC sectional aerosol module (Zaveri et al., 2008). We have added the CRIMEch gas phase chemistry scheme (Watson et al., 2008) to WRF-Chem using the KPP interface, and coupled it to the MOSAIC sectional aerosol module. In addition we have modified MOSAIC to include the heterogeneous uptake of N₂O₅ (Bertram & Thornton, 2009). The details of these, and other, developments made to WRF-Chem are covered in a companion presentation.

Anthropogenic emissions have been calculated using the NAEI (naei.defra.gov.uk) and TNO (Denier van der Gon et al., 2010) emission databases, with diurnal and weekly cycles superimposed. Biogenic emissions are calculated online within WRF-Chem, based on USGS land-use categorisation. The meteorological fields are initialised with, and bounded by, ECMWF ERA Interim data (Dee et al., 2011) Radiative feedback from the aerosol fields is allowed to influence the meteorology. Chemical boundary conditions are taken from MOZART global model data (Emmons et al., 2010).

Three chemical scenarios are considered: a base case with full N₂O₅ heterogeneous chemistry; N₂O₅ heterogeneous chemistry without the chloride ion pathway; and no N₂O₅ heterogeneous chemistry. For each scenario we have run the model over a 15km resolution grid covering NW Europe for the period 10–30th July 2010. A second domain, covering England and the North Sea at a

resolution of 5km, has also been run for selected dates during this period for more detailed comparisons with aircraft measurement data.

We will present an analysis of the effects of N₂O₅ heterogeneous chemistry on: i) night-time gas-phase NO_x chemistry; ii) the regional distribution of aerosol composition; iii) the relative day-time and night-time contributions to nitrate aerosol and of the relative contribution of the hydrolysis and chloride channels to the effects.

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