Coupled chemical mechanism and sectional aerosol developments within WRF-Chem

D. Lowe[1], S. Archer-Nicholls[1], S. Utembe[1,2], D. Topping[1,3], M. Barley[1], R. Zaveri[4], G. McFiggans[1]

[1]Centre for Atmospheric Science, University of Manchester, Manchester, M13 9PL, United Kingdom
[2]Earth Sciences, The University of Melbourne, Victoria, Australia
[3]National Centre for Atmospheric Science, University of Manchester, Manchester, M13 9PL, United Kingdom
[4]Pacific Northwest National Laboratory, Richland, Washington, USA
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Presenting author email: douglas.lowe@manchester.ac.uk

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 also influence the climate, directly through radiative scattering and adsorption, and indirectly through influencing cloud formation by acting as cloud condensation nuclei. In order to improve our understanding of how aerosols have these effects they have been included, with varying degrees of detail, in global and regional atmospheric models.

The mesoscale Weather Research and Forecasting (WRF) meteorological model (http://www.wrf-model.org; Skamarock et al., 2005) has been expanded to create the WRF-chem model (Grell et al., 2005), which simulates gas-phase chemical and aerosol microphysical processes on-line with the meteorological fields, allowing explicit coupling between the processes. A variety of gas-phase chemical schemes and aerosol mechanisms are available and the modular setup of WRF-chem allows different gas-chemistry and aerosol modules to be evaluated and compared using the same chemical emissions and meteorology input data (c.f. Fast et al., 2006). Here we present developments made to WRF-chem with the aim to improve the representation of gaseous and condensed-phase processes for use within, and to address the scientific objectives of, the NERC funded RONOCO and VOCALS-UK consortium projects.

We have extended the gas-phase chemistry options by adding the CRIv2 (Common Representative Intermediates, version 2) gas-phase scheme (Watson et al., 2008). This is derived from the Master Chemical Mechanism, and enables improved modelling of organic gas-phase chemistry, which is important in reproducing ozone and the volatile organic compound (VOC) budgets.

The MOSAIC aerosol module (Zaveri et al., 2008) has been extended with the addition of organic aerosol components, comprising of 2 involatile, and 13 semi-volatile, organic compounds (Barley et al., 2011). Non-ideal interactions between these compounds in the condensed-phase, which change the individual component vapour pressures, are calculated using the PD-FiTE method (Topping et al., 2012). The partitioning organic components have been chosen using MCM box-model studies to select the greatest contributing components to organic aerosol mass. These have been linked either to related CRIv2 compounds or, where no suitable compounds exist, related to the concentrations of surrogate compounds through numerical fits.

Sea-spray aerosol source terms have been updated following the work of Fuentes et al. (2010; 2011). This extends the source term down to smaller particle sizes and connects the source term to the biogenic activity of the ocean, allowing the representation of the influence of the organic content on particle formation. Also included is a size-resolved primary organic fraction to the sea-spray emissions, assumed involatile.

Night-time NOx chemistry and aerosol formation is governed by the heterogeneous uptake of N_2O_5 on aerosol particles. We have incorporated the parameterisation of Bertram and Thornton (2009) into the MOSAIC sectional aerosol module to represent this process. This converts N_2O_5 to aerosol nitrate and $ClNO_2$, with composition dependent uptake coefficients and branching ratios.

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