Modelling Ozone in the Lower Troposphere

Ground-level ozone interacts with plants and with other pollutants. These interactions are highly non-linear and may enhance or deplete ground-level ozone so need to be properly represented by models. Model domains and scales (vertical and horizontal) are key limitations for the simulation of ground-level ozone. In areas with high emissions of nitrogen oxides (NOₓ, i.e. large cities) reaction with NOₓ plays a major role in controlling ground-level ozone, whereas in less polluted areas hemispheric transport is a major driver of ground-level ozone. Biogenic emissions are also a critical source of biogenic volatile organic compounds (VOCs) which are precursors of ozone formation.

The figure below shows annual average surface ozone for the year 2008 calculated by the EMEP4UK model. Left panel shows the European domain at a 50 km x 50 km horizontal resolution and the right panel shows the UK domain at a 5 km x 5 km horizontal resolution.

Key Facts

- As ozone is formed by the chemical transformation of precursor emissions (mainly nitrogen oxides and non-methane volatile organic compounds) which are spatially and temporally highly variable, models are an essential tool to investigate and understand current and future ozone levels.

- Global climate change and interaction effects with air pollution need to be modelled at different spatial scales in order to adequately represent the atmospheric processes driving these changes.

Links

- www.defra.gov.uk
- www.epa.gov
- www.ncas.ac.uk
- ncar.ucar.edu
- www.emep.int
- www.ipcc.ch
- www.emep4uk.ceh.ac.uk
Recent developments

The availability of more powerful computers allows researchers to perform simulations at relatively high resolution - both in space and time - for the entire globe in order to better represent the chemistry interaction in areas with high concentrations of nitrogen oxides (NO\textsubscript{X}, the sum of NO and NO\textsubscript{2}).

Atmospheric chemistry transport models can now be applied from global to local scales in a nested approach for large geographical domains, providing a consistent model simulation from the coarse (global) to the fine scale (for instance a large city).

This improved spatial resolution is required to model more accurately the photo-chemistry associated with ozone formation and reaction with NO which happens on timescales of minutes and which cannot be adequately simulated in large spatial grids; yet the large spatial domains are still essential in order to capture the ozone processes, including hemispheric transport, that happen on days/weeks timescales and act on regional scales.

The climate and atmospheric chemistry interactions can now be explored with fully coupled meteorology and chemistry models at regional and local scales. The meteorology and climate variables can affect all aspects of ozone processes (emissions, transport, chemistry, deposition), meaning that substantial uncertainties remain. Current developments e.g. in the area of Earth System Modelling (ESM) can be utilised to reduce these uncertainties.

What is needed?

- Emissions are a major uncertainty in modelling ozone, especially, but not only, biogenic emissions of volatile organic compounds (VOCs).
- Global scale models well represent hemispheric transport of ozone, but not highly polluted areas. The effects of small scale interactions on large scale tropospheric ozone are uncertain. Ground level emissions of ozone precursors e.g. within street canyons need to be calculated with the appropriate dispersion model at high resolution.
- Exchange between the stratosphere and troposphere may be important in the future and is so far not always included in air quality models.
- Observation networks, both in the UK and elsewhere, are designed to provide observations for regulatory purposes, and are not always adequate for model validation purposes.
- Increases in model complexity make it difficult to interpret comparisons among different models, requiring the development of new metrics and criteria for the assessment of model output quality.

The Ozone Challenge

Ozone is formed in the lower atmosphere by the action of sunlight on nitrogen dioxide (NO\textsubscript{2}), which is naturally present from lightning, biomass burning and soil emissions; man-made contributions to NO\textsubscript{2} from burning fossil fuels dominate in developed regions. Ozone formation is accelerated by the presence of organic gases, both biogenic and man-made. Ozone is toxic to plants, animals and humans; toxic concentrations are found in polluted air, downwind of NO\textsubscript{2} sources and especially in strong sunlight. Ozone is removed from the atmosphere by deposition to plants, and also by reaction with nitric oxide (NO) to form NO\textsubscript{2}.

Further information and contact details:
www.ozone-net.org.uk

Other Fact sheets in the series:
- Ozone monitoring
- Health effects of ozone
- Ecosystem effects of ozone
- Agricultural and crop-effects of ozone