Chemistry and aerosol modelling with the UM
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Air Quality and Composition Team, Met Office, UKCA team
A talk of two halves – the outline

• Part 1. Aerosols, past, present and future
  • Aerosol schemes available in the UM
  • Past/current applications
  • Future plans

• Part 2. UKCA – the future of chemistry and aerosol modelling in the UM
  • What is UKCA?
  • What can it do?
Met Office Aerosol schemes – past, present and future
Nick Savage
Why do we care? (1)
Radiation, clouds and precip

Figure 2.10 from Climate Change 2007: Working Group I: The Physical Science Basis, Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M. Tignor and H.L. Miller (eds.)
Data from SINERGEE project using 6Z, 12Z, 18Z, 24Z, July 2003

The +ve anomaly over desert is ~ -ve anomaly over ITCZ clouds

c/o Jim Haywood
Why do we care (3)? Visibility, Human Health

Claude Monet, London, Houses of Parliament. The Sun Shining through the Fog

Cartoon courtesy of New Zealand Ministry for the Environment

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Available aerosol schemes
Representations of aerosol in the UM

• 1D land/sea Climatologies
• 3D Climatologies
• Single advected tracer: ‘Murk’
• CLASSIC: bulk aerosol scheme
• UKCA-GLOMAP-mode. Modal aerosol scheme

Increasing complexity, increasing cost
1D/3D climatologies

- **Very Cheap**
- **Cusack 1D Climatology**
  - Based on assumption that Land = Polluted, Sea = Clean
  - One profile for land, one for sea
  - Mostly used in NWP for radiative effects
- **3D climatologies**
  - Monthly means of model using CLASSIC aerosol scheme
  - Read in from Ancil files
Murk

• 1 tracer “anthropogenic” aerosol
• Represents emissions, transport and wet deposition of tracer
• Used in UKV forecast model for visibility prediction and in data assimilation
• Visibility parameterised as a function of aerosol concentration and total water
• DA uses murk as a control variable
• Autoconversion also linked to murk
CLASSIC aerosol scheme

- Sulphate, Black Carbon, Organic Carbon, Sea Salt, Biomass Burning, Dust (2 or 6 bins), Nitrate (only available with UKCA chemistry on)
- External mixtures (components are treated separately)
- Emissions either specified (e.g. CMIP5, AEROCOM) or a function of the model meteorology (sea-salt, mineral dust)
- Transport, chemical transformation, wet-deposition, dry deposition of aerosols (except sea-salt)
- Treats direct and indirect radiative effects
- Fixed size distribution for each aerosol type
UKCA-GLOMAP-mode

- Developed in partnership by Met Office, Cambridge, Leeds and Oxford Universities
- Both number and mass are prognostic
- Internally mixed
- 7 modes (4 soluble, 3 insoluble)
- 39 tracers
- More in part 2
Aerosol schemes used in key Met Office configurations

• UKV model:
  • Murk for visibility and autoconversion
  • 1D Climatology for radiation

• Global Atmosphere (GA5):
  • Climate: CLASSIC (not nitrate), 6-bin dust
  • Global NWP: 3D climatologies + 2-bin CLASSIC dust

• UK Air Quality forecast (AQUM):
  • CLASSIC (including nitrate) plus UKCA chemistry
Mineral dust data assimilation

Yaswant Pradhan, Bruce Ingleby

- Global NWP model
- MODIS AOD data
- 4D-Var
- Operational in PS 32
- Mainly adding dust, except Sahara. Better fit to AERONET.
Simple Land/Sea climatologies

Improved CLASSIC aerosol climatologies

Replacement of climatologies with prognostic schemes based on CLASSIC
- Sea-salt
- Biomass burning

Reasonable monthly means but no relation to meteorology

Fully prognostic driven by meteorology

2001-2008
Met Office

Little resemblance to reality

2008-2011

Current

Mid-Term Upgrades
MACC/GEMS Assimilated aerosol for initial conditions
Prognostic UKCA - GLOMAP - mode
DA of fires for biomass burning

c/o Jim Haywood

2001-2008

Little resemblance to reality
Other medium term plans

- Global climate modelling
  - Move to using UKCA-GLOMAP-mode (in progress)
- UK Air Quality
  - Move to using UKCA-GLOMAP-mode
- UK NWP models (longer term)
  - Reduced complexity UKCA-GLOMAP-mode
  - Visibility: will need data assimilation and more work
More information

- CLASSIC Documentation paper UMDP 20 (on collaboration wiki) and Bellouin et al 2012, DOI: 10.1029/2011JD016074
  - includes some information on 3D aerosol climatologies
- Murk: Clark et al (2008), QJRMS
Questions and answers
UKCA
Nick Savage and UKCA team

Air Quality and Composition Team, Met Office, UKCA team

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Outline

• What is UKCA?
• Chemical mechanisms
• GLOMAP-mode Aerosol scheme
• Applications
• More information
What is UKCA?

- **United Kingdom Chemistry and Aerosols**
- A Chemistry **and** Aerosol scheme for the Met Office Unified Model
- Funding from National Centre for Atmospheric Science (NCAS) and the Met Office
- Not a single model
  - framework for composition modelling
  - gives the user multiple options for chemistry and for aerosols
Participants

- Met Office: Tropospheric Chemistry, direct radiative forcing, system management...
- University of Cambridge: Stratospheric Chemistry, wet deposition, photolysis...
- Leeds University: Aerosol Scheme
- Oxford: indirect effects of aerosols and aerosol washout
- Funding from JWCRP
Highly coupled to rest of UM

Figure courtesy of N. Luke Abraham (NCAS/University of Cambridge)
Chemical mechanisms and photolysis
What is a chemical mechanism?

1. List of reactions
2. How quickly reactions proceed

Figure courtesy of Alex Archibald, Cambridge University
Chemical mechanisms - why not only one?

- Only one ‘real’ atmospheric chemistry!
- more complex mechanism = more expensive
- chemistry already most expensive part of model if on
- Master chemical mechanism:
  - 17000 reactions
  - 6700 species
- choose a small subset of these
- Choice of reactions depends on application
Chemical mechanisms in UKCA

- TropIsop (CHET). Simple tropospheric scheme with isoprene. 31 tracers, 167 reactions
- Strat (CHES). Represents the chemistry of the stratosphere for use in studies of stratospheric ozone (e.g. $O_3$ hole recovery). 37 tracers, 169 reactions
- StratTrop (CHEST). Represents the chemistry in the troposphere and stratosphere, to be used in next ESM, 71 tracers, 283 reactions
- Regional Air Quality (RAQ) – more VOCs than TropIsop, used in operational AQ forecasting model. 40 tracers, 215 gas-phase reactions
Photolysis schemes

- Photolysis is the process where molecules are split apart by light
- Key part of atmospheric chemistry
- UKCA offers three schemes:
  - Simple interpolation from 2D data. Used in HadGEM2-ES. Cheap but uses climatological cloudiness not modelled Liquid Water Content (LWC)
  - Fast-J. Photolysis scheme coupled to modelled LWC. Used in AQUM. Unsuitable for stratospheric modelling, retirement now planned.
  - Fast-JX. Upgraded version of Fast-J with more wavelength bands so can be used for stratosphere as well as troposphere
GLOMAP-mode Aerosol scheme
UKCA-GLOMAP-mode (c/o Graham Mann)

7 internally mixed modes – number in each mode is a prognostic variable

Aerosol mass tracked for:
**Sulphate, sea salt, black carbon, organic carbon, dust**

3 insoluble modes

- Insoluble Aitken
  - N5
  - BC OC

- Insoluble accum
  - N6
  - DU

- Insoluble coarse
  - N7
  - DU

4 soluble modes

- Soluble nucln
  - N1
  - SO4 OC

- Soluble Aitken
  - N2
  - SO4 BC

- Soluble accum
  - N3
  - SO4 BC CI DU

- Soluble coarse
  - N4
  - SO4 BC CI DU

7 internally mixed modes – number in each mode is a prognostic variable.
UKCA-GLOMAP-mode Aerosol Scheme

• Can be configured to use different subsets of the modes and the components in each mode

• Aerosol sources include:
  - direct emissions from anthropogenic and biogenic sources
  - wind driven emissions (dust and sea-salt)
  - nucleation
  - gas to particle conversion from SO$_2$ and SOA

• Direct and indirect effects of aerosols can be included

• Work to add ammonium nitrate is in progress
UKCA-GLOMAP-mode – Chemistry schemes

- Include SO$_2$, DMS, H$_2$SO$_4$ and monoterpenes etc to produce condensable products
- Available as an add on to some chemistry schemes
- Oxidation processes modelled explicitly
- Aqueous oxidation rates provide in-cloud growth rates of aerosol
- H$_2$SO$_4$ concentrations used for nucleation and deposition to aerosol
UKCA-GLOMAP-mode Annual mean (Graham Mann)

Nucleation mode N

Aitken mode N

Condensation nuclei

CCN

Cloud condensation nuclei (cm$^{-3}$)

Number conc (per cc)

0.1

0.2

0.5

1.0

5.0

10.0

20.0

50.0

100.0

200.0

500.0

1000.0

2000.0

5000.0

10000.0

0

5

10

15

20

25

30

0

-50

0

50

Latitude

Altitude (km)

CCN (acc.
rate < 0.029CCN)

Concen. (cm$^{-3}$)

1

2

5

10

20

50

100

200

500

1000

2000

5000

10000
Applications of UKCA
Air quality Modelling
Nick Savage, Paul Agnew, Lucy Davis, Carlos Ordonez, Marie Tilbee
Air Quality in the Unified Model - AQUM

- Operational model, 5 day forecast, run daily
- Meteorological BC from Met Office Global model
- Chemical and aerosol BC from MACC-II real time forecasts
- Uses RAQ chemistry scheme, CLASSIC aerosol
- Post-processing includes bias correction using observations from the national monitoring network
Near-real-time verification

- We conduct routine verification against observations from the UK Automatic Urban and Rural Network (AURN)
  - Surface measurements of O3, NO2, NO, CO and PM are available
- This provides a rapid method of evaluating the forecast on a daily basis
- Constant objective evaluation aids our model development
Wednesday 25th July – week before Olympics opening ceremony
New Earth System Model

Fiona O’Connor
Earth System Model

**PHYSICAL CLIMATE**

- Radiation, cloud
- Radiation & cloud through photolysis
- Greenhouse Effect

**GREENHOUSE GASES**

- CO₂, N₂O

**LAND**

- O₃ damage, N Deposition
- Wetland CH₄, dry dep, stomatal uptake, BVOCs, N emissions

**AEROSOLS**

- SO₄²⁻, NO₃⁻, SOA formation
- Heterogeneous chemistry, photolysis
- DMS, dust, emissions
- CH₄, N₂O, CFCs, trop & strat O₃

**ECOSYSTEMS**

- C&N cycles

**CHEMISTRY** (trop & strat)

**LAND ICE**

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New Earth System Model
UK-ESM1

• Collaboration with NERC

• Whole atmosphere chemistry (stratosphere and troposphere)

• Interactive Biogenic VOC

• Fast-JX interactive photolysis scheme

• GLOMAP-mode aerosols (including nitrate and dust)

• Direct and indirect effects of aerosols
Progress so far (1)

Zonal mean ozone From Fiona O’Connor

Model: UKCA (20-year monthly mean)
Obs: NIWA climatology (Hassler et al. 2009)
Progress so far (2)

MODE Aerosols with Offline Chemistry
From Colin Johnson

Aim: Replace the CLASSIC aerosol scheme in HadGEM3-A with UKCA-MODE aerosols
More information

- Documentation paper UMDP 84 (on collaboration wiki)
- UKCA website: [http://www.ukca.ac.uk/](http://www.ukca.ac.uk/)
- Mohit Dalvi supports UKCA at Met Office
- Luke Abraham (University of Cambridge) supports UKCA for NERC community
- UKCA tutorial in development, funded by ACITIES
Questions and answers

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Additional slides
Code management
Code management

- At vn8.2 much of the NCAS community code lodged to the trunk
  - Required major effort to merge code at vn7.3 and then update to to vn8.1
  - Not sustainable process
- New aim is an approach where jobs shared between Met Office and partners are updated annually
- First jobs to be released soon (currently being evaluated)
- New code to be brought in as soon as possible as separate code branches, developed at latest annual release
- Testing and review prior to agreement by Met Office to lodge
Inputs to UKCA from other parts of MetUM

- Physical variables e.g. PRESSURE AT RHO LEVELS, PV on model theta levels
- Radiation - NET DOWN SURFACE SW FLUX and TOTAL DOWNWARD SURFACE SW FLUX
- Boundary layer e.g. Turbulence diagnostics, SURFACE HEAT FLUX, resistances for dry deposition
- Cloud related e.g. CLOUD LIQUID WATER
- Precip related e.g. RAINFALL RATE
- Natural emissions from vegetation scheme (not lodged)
Inputs to other MetUM schemes from UKCA

- Trace gases in radiation schemes
- Oxidants from UKCA may be coupled to CLASSIC sulphur oxidation scheme (and CLASSIC can deplete)
- Direct radiative effect of MODE aerosols (RADAER)
- Indirect radiative effect of MODE aerosols (code to couple to cloud scheme not lodged, only code to calculate CCN)