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

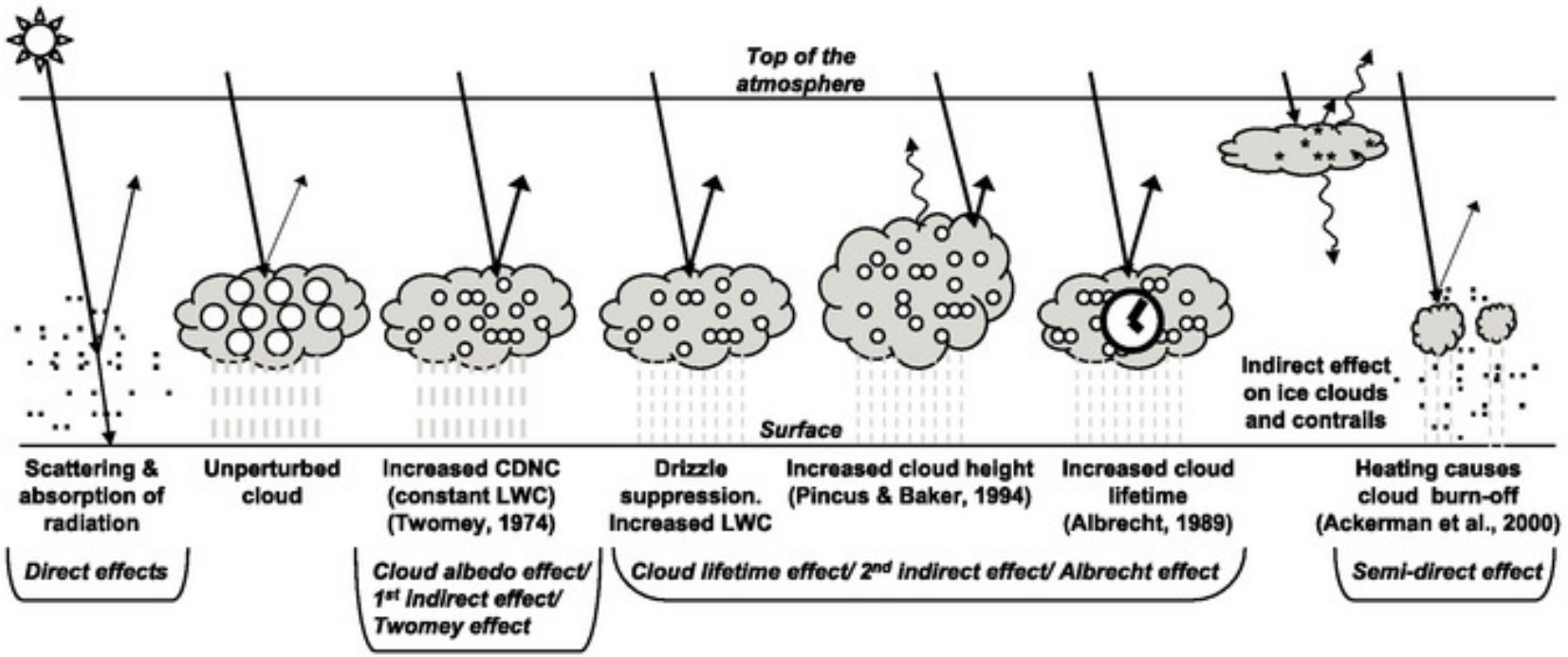
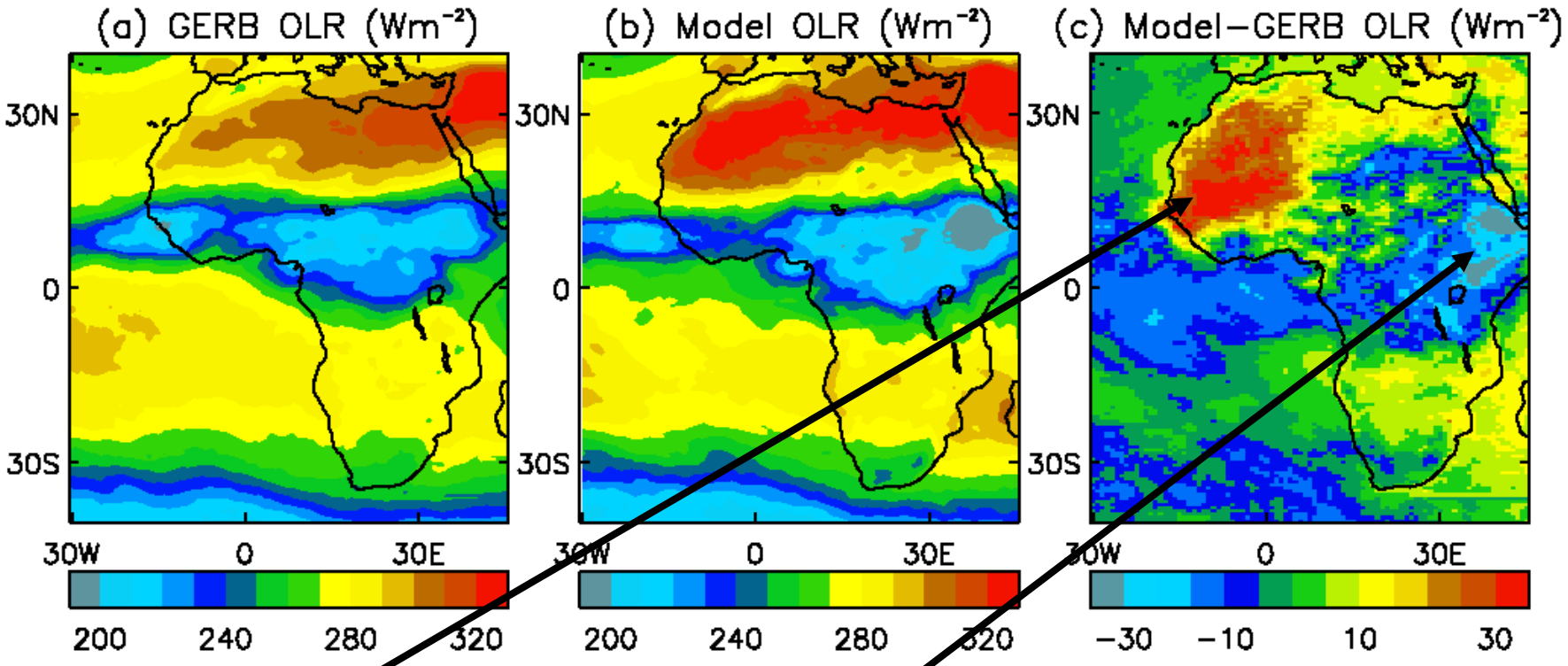


Figure 2.10 from Climate Change 2007: Working Group I: The Physical Science Basis, Solomon, S., D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Averyt, M. Tignor and H.L. Miller (eds.)

Why do we care (2)?

Data from SINERGEE project using 6Z, 12Z, 18Z, 24Z, July 2003



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

c/o Jim Haywood

Why do we care (3)? Visibility, Human Health

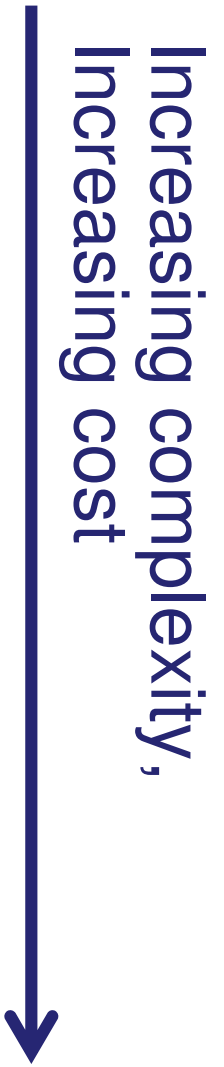
Claude Monet, London, Houses of Parliament. The Sun Shining through the Fog

Cartoon courtesy of New Zealand Ministry for the Environment

Available aerosol schemes

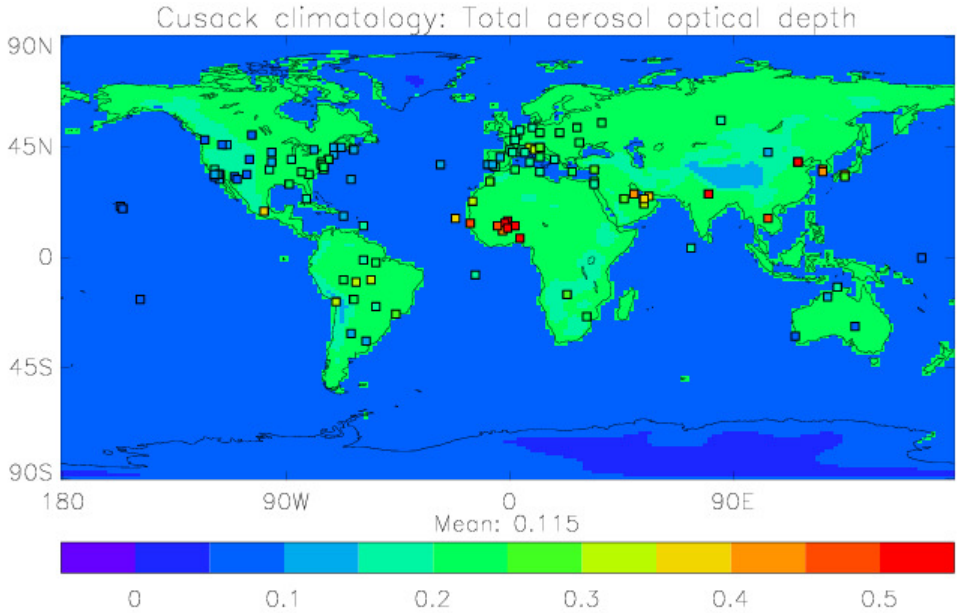
Representations of aerosol in the UM

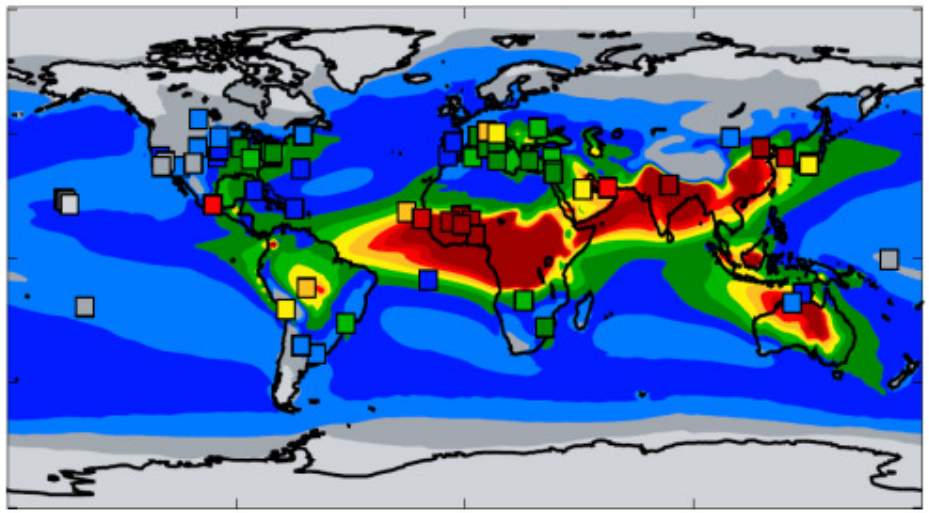
- 1D land/sea Climatologies
- 3D Climatologies
- Single advected tracer: ‘Murk’
- CLASSIC: bulk aerosol scheme
- UKCA-GLOMAP-mode. Modal aerosol scheme



1D/3D climatologies

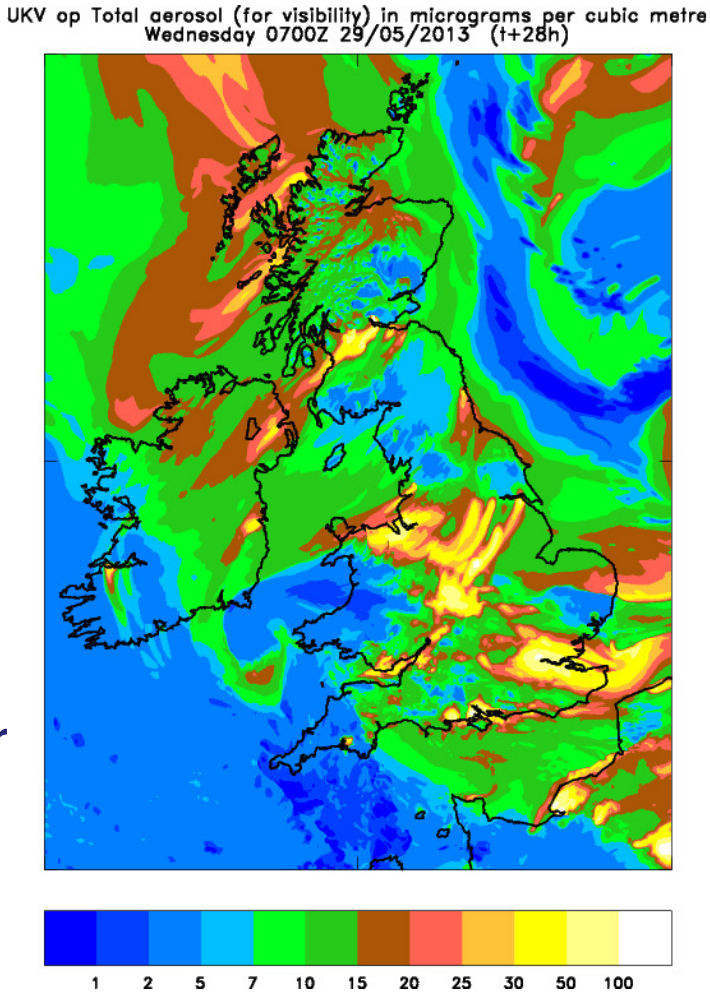
- Very Cheap
- Cusack 1D Climatology
  - Based on assumption that Land=Polluted, Sea = Clean
  - One profile for land, one for sea
  - Mostly used in NWP for radiative effects
- 3D climatologies
  - Monthly means of model using CLASSIC aerosol scheme
  - Read in from Ancil files





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 a function of aerosol concentration and total water
- DA uses murk as a control variable
- Autoconversion also linked to murk

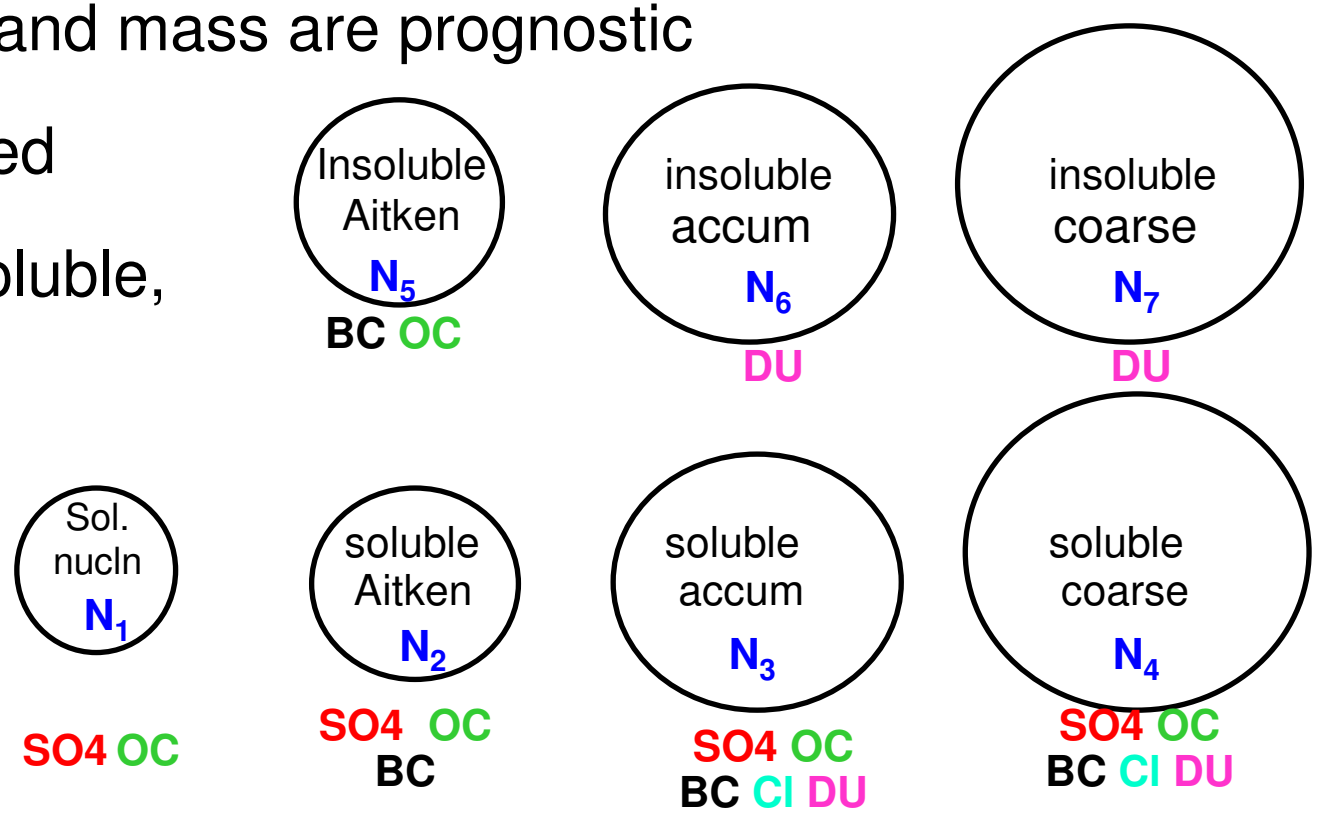


CLASSIC aerosol scheme

- 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



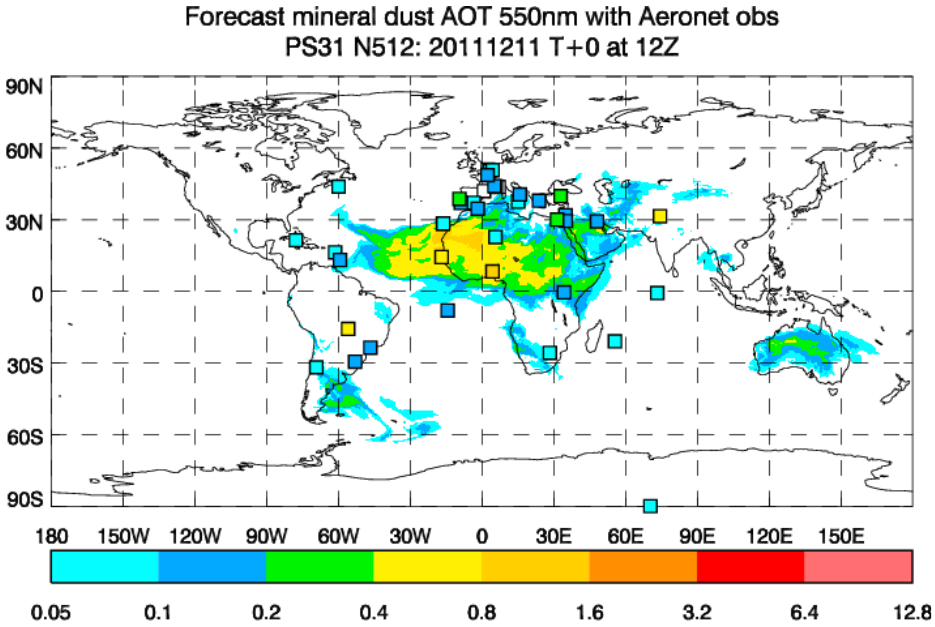
Aerosol schemes used in key Met Office configurations

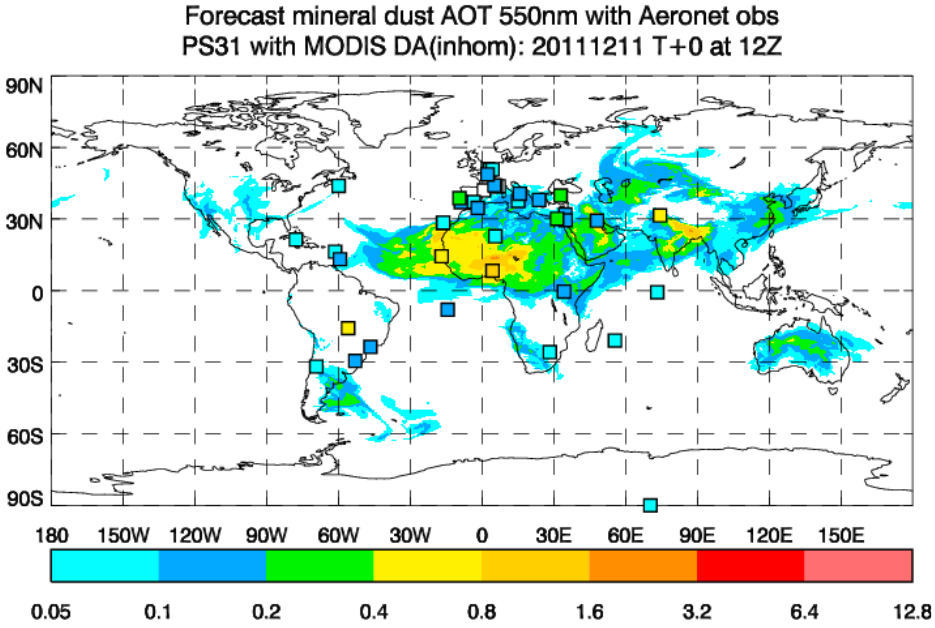
- UKV model:
  - Murk for visibility and autoconversion
  - 1D Climatology for radiation
- Global Atmosphere (GA5):
  - Climate: CLASSIC (not nitrate), 6-bin dust
  - Global NWP: 3D climatologies + 2-bin CLASSIC dust
- UK Air Quality forecast (AQUM):
  - CLASSIC (including nitrate) plus UKCA chemistry

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.

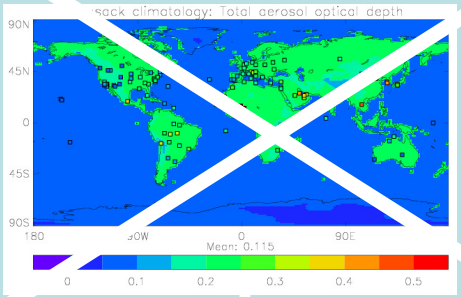




2001-2008

Met Office

Simple Land/Sea climatologies

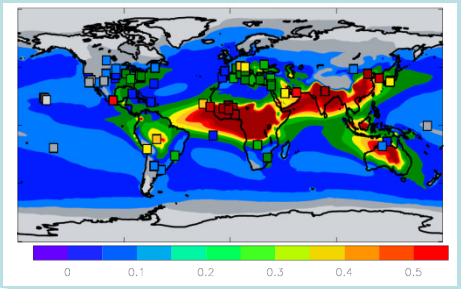


Little resemblance to reality

c/o Jim Haywood

2008-2011

Improved CLASSIC aerosol climatologies



Reasonable monthly means but no relation to meteorology

Current

Replacement of climatologies with prognostic schemes based on CLASSIC

- Saharan dust* (2011) + DA* (2013)
- Sea-salt
- Biomass burning

Fully prognostic driven by meteorology

Mid-Term Upgrades

MACC/GEMS Assimilated aerosol for initial conditions

Prognostic UKCA - GLOMAP - mode

DA of fires for biomass burning

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

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

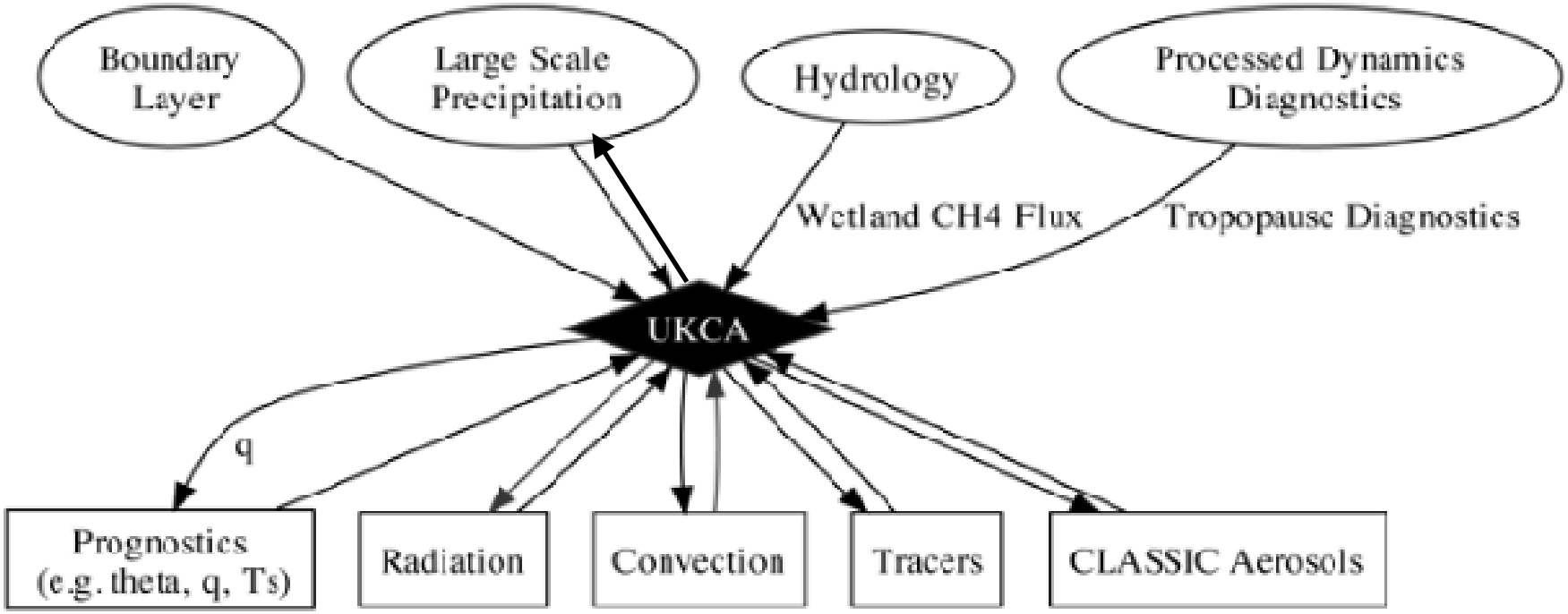


Figure courtesy of N. Luke Abraham (NCAS/University of Cambridge)

Chemical mechanisms and photolysis

What is a chemical mechanism?

1.List of reactions

2.How quickly reactions proceed

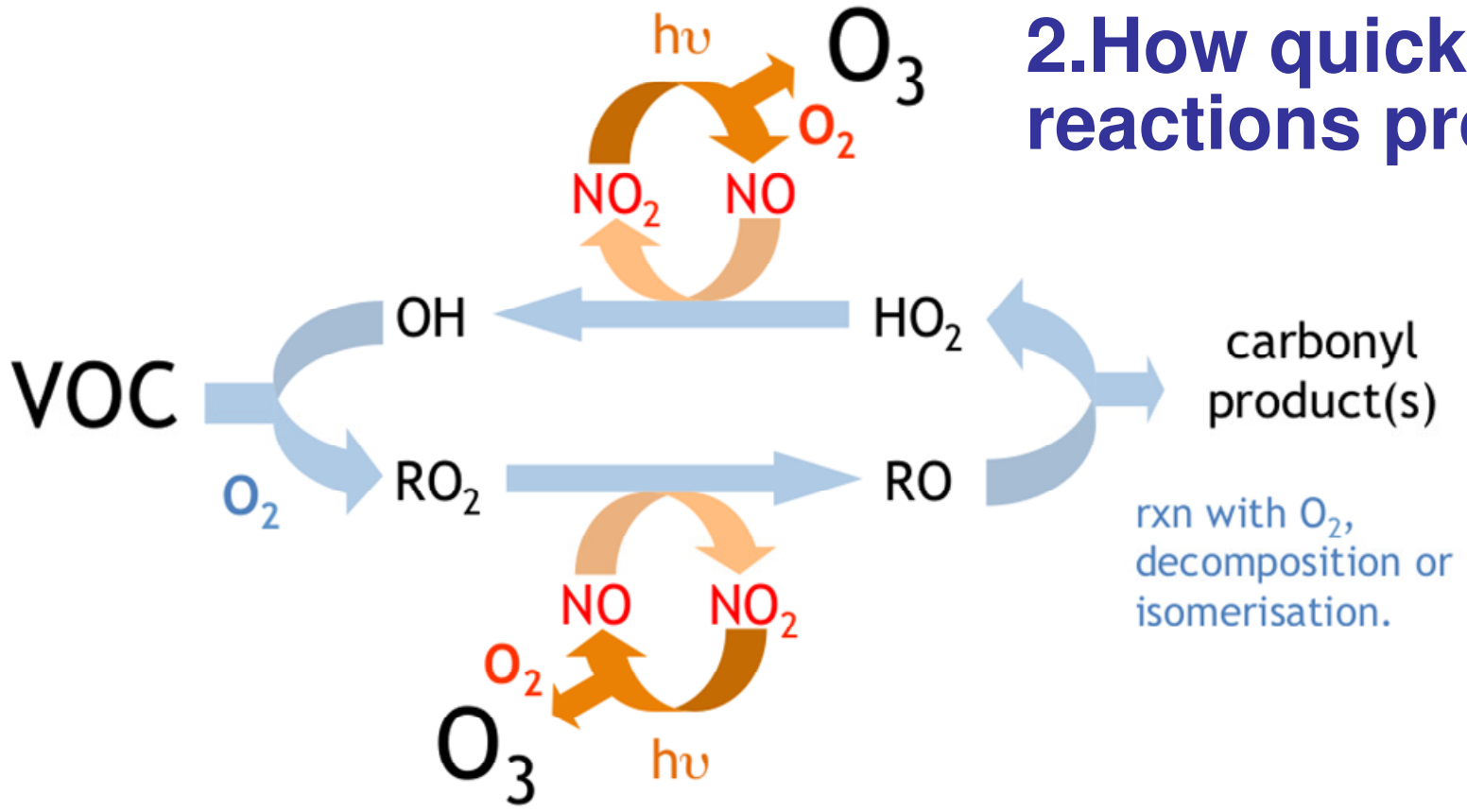


Figure courtesy of Alex Archibald, Cambridge University

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 be 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

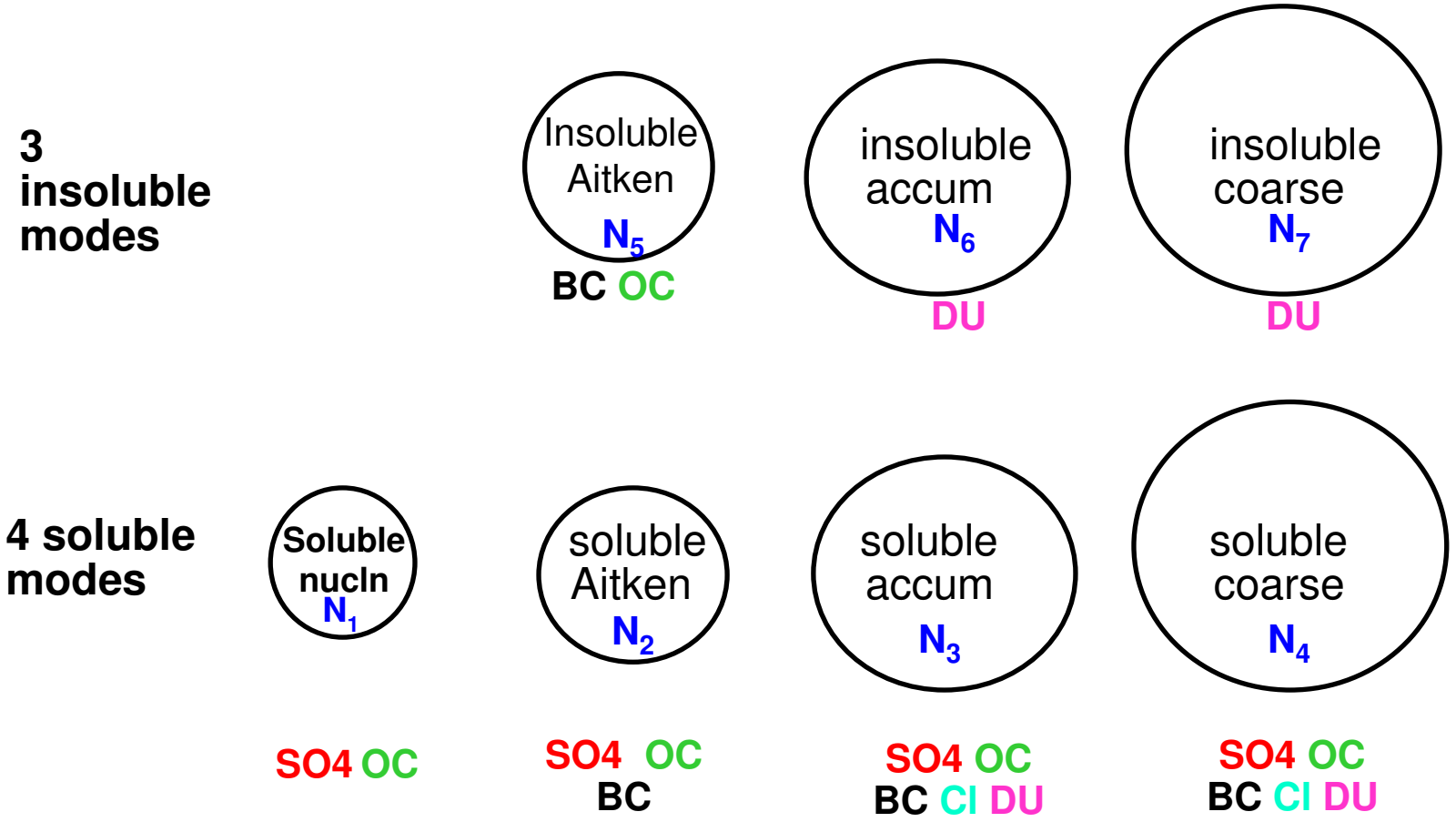
GLOMAP-mode Aerosol scheme

UKCA-GLOMAP-mode (c/o Graham Mann)

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

Aerosol mass tracked for:

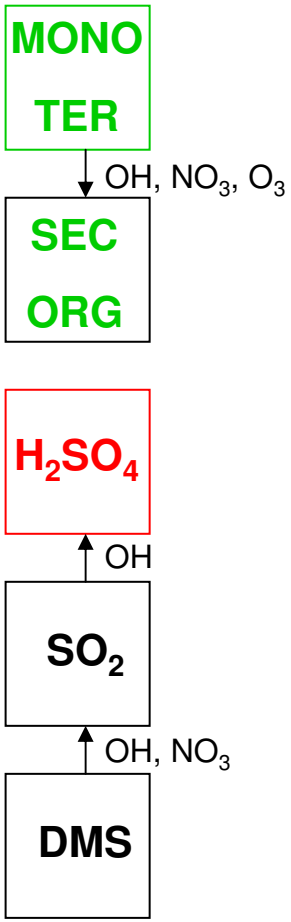
Sulphate, sea salt, black carbon, organic carbon, dust



UKCA-GLOMAP-mode Aerosol Scheme

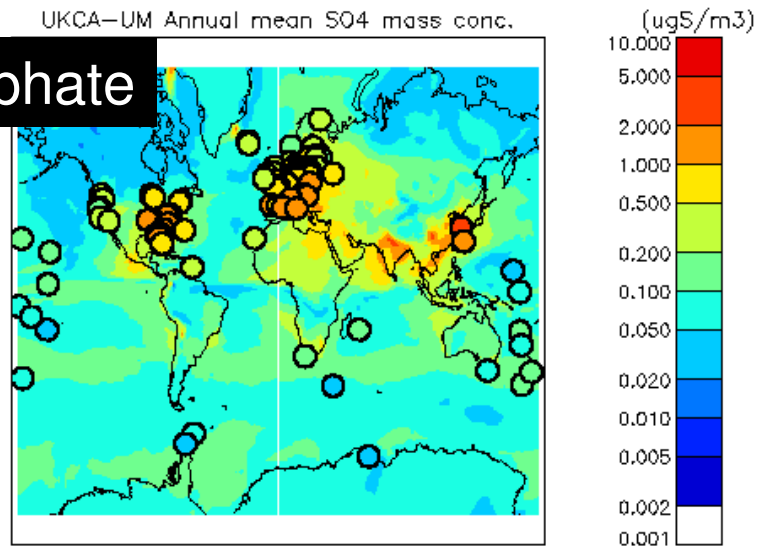
- Can be configured to use different subsets of the modes and the components in each mode
- Aerosol sources include:
  - direct emissions from anthropogenic and biogenic sources
  - wind driven emissions (dust and sea-salt)
  - nucleation
  - gas to particle conversion from SO_2 and SOA
- Direct and indirect effects of aerosols can be included
- Work to add ammonium nitrate is in progress

UKCA-GLOMAP-mode – Chemistry schemes

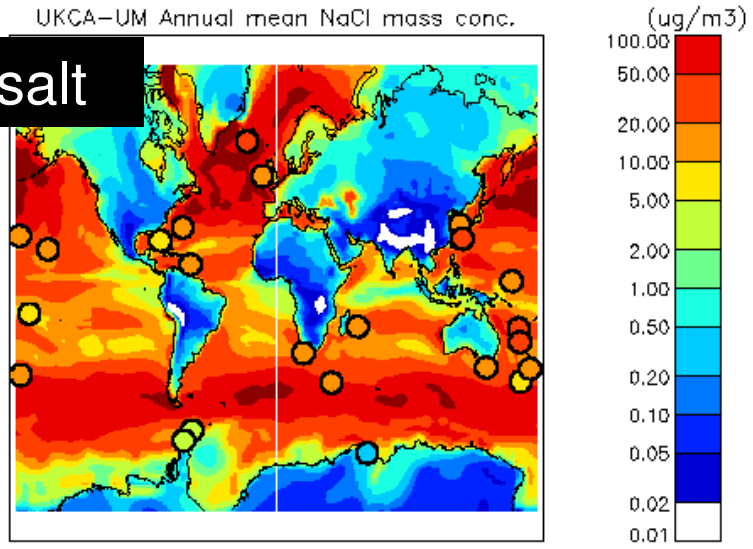


- Include SO_2, DMS, H_2SO_4 and monoterpenes etc to produce condensable products
- Available as an add on to some chemistry schemes
- Oxidation processes modelled explicitly
- Aqueous oxidation rates provide in-cloud growth rates of aerosol
- H_2SO_4 concentrations used for nucleation and deposition to aerosol

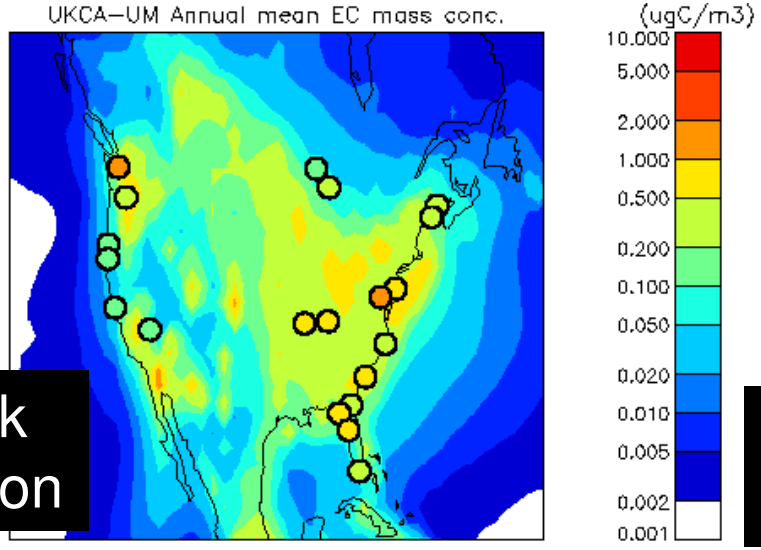
UKCA-GLOMAP-mode Annual mean (Graham Mann)



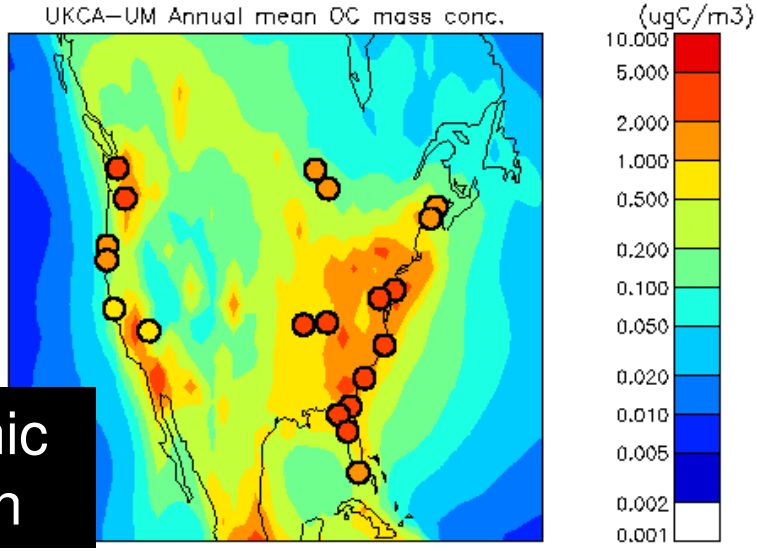
Sulphate



Sea salt

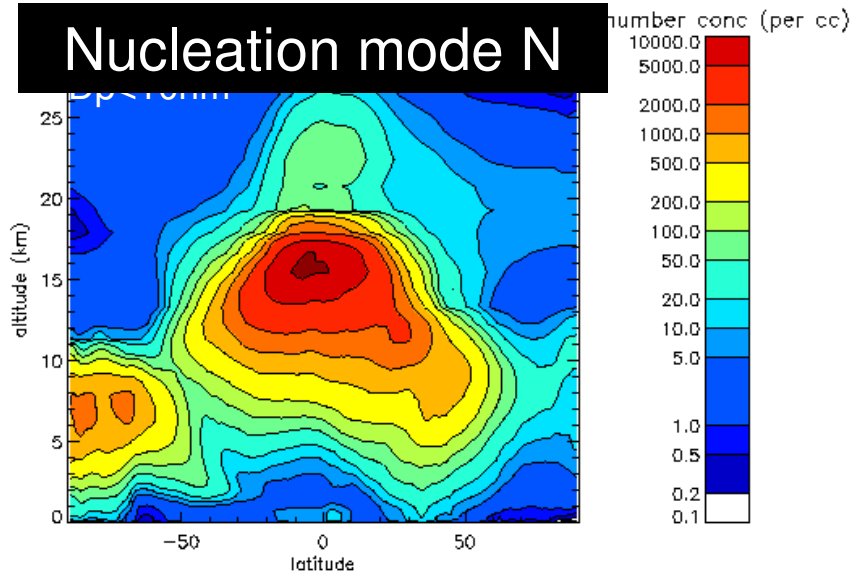


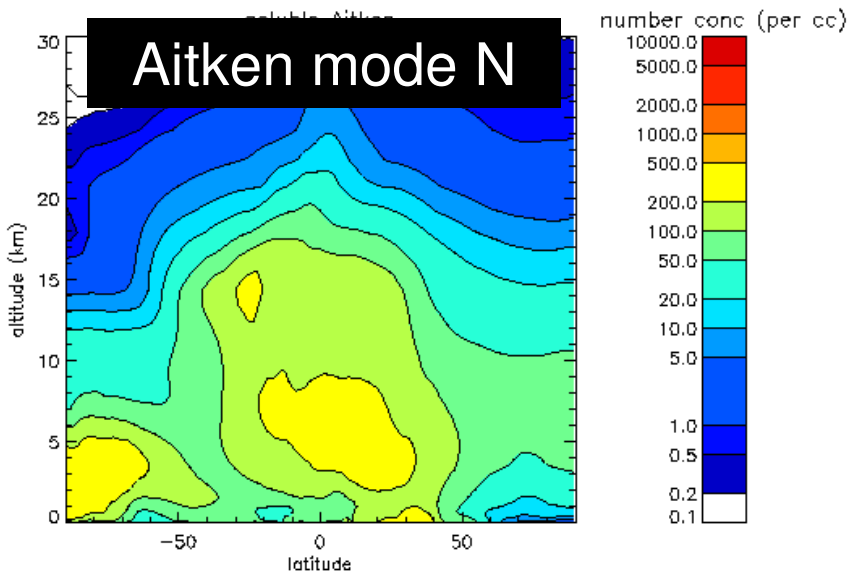
Black carbon

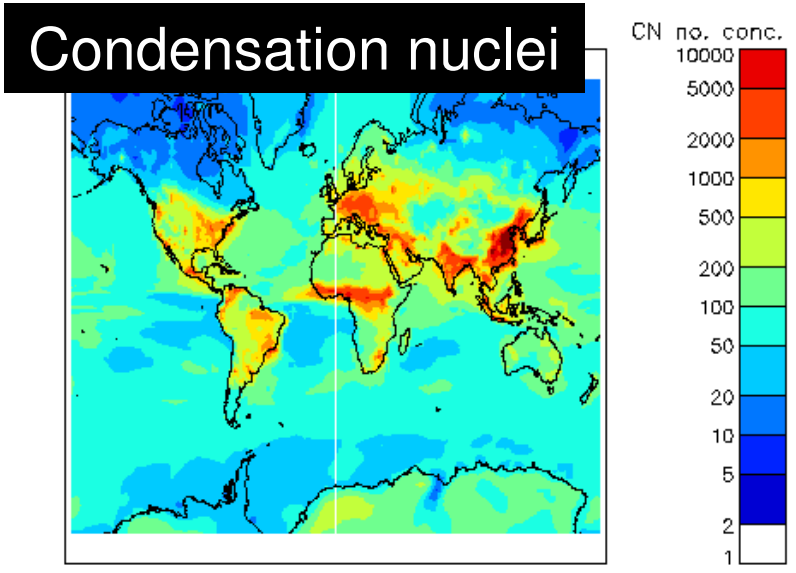


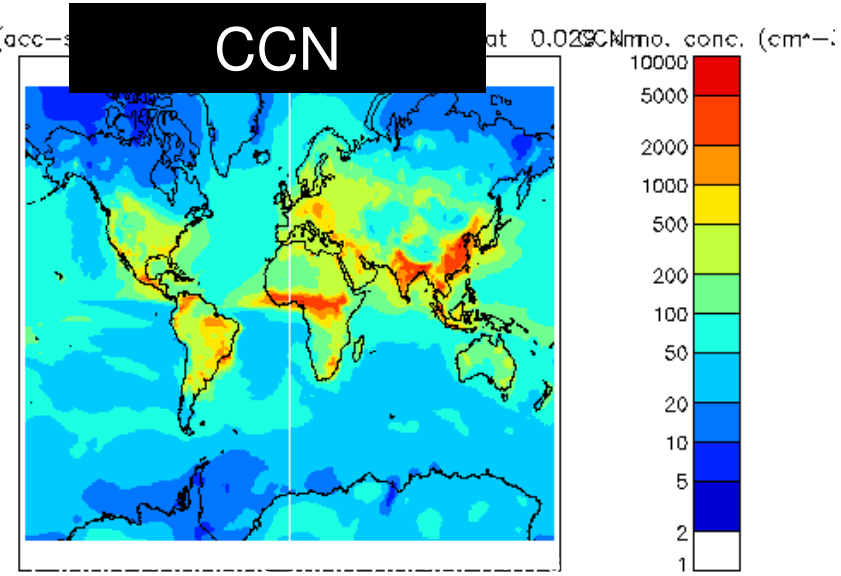
Organic carbon

UKCA-GLOMAP-mode Annual mean (Graham Mann)









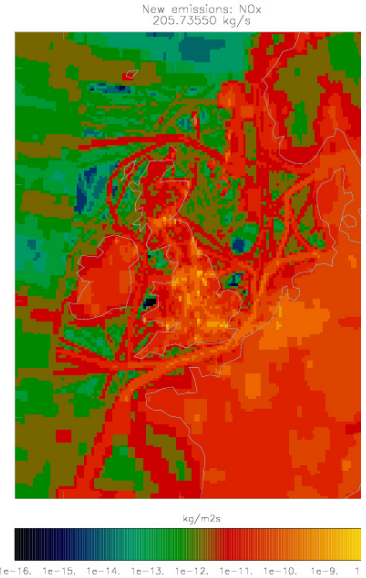
Applications of UKCA

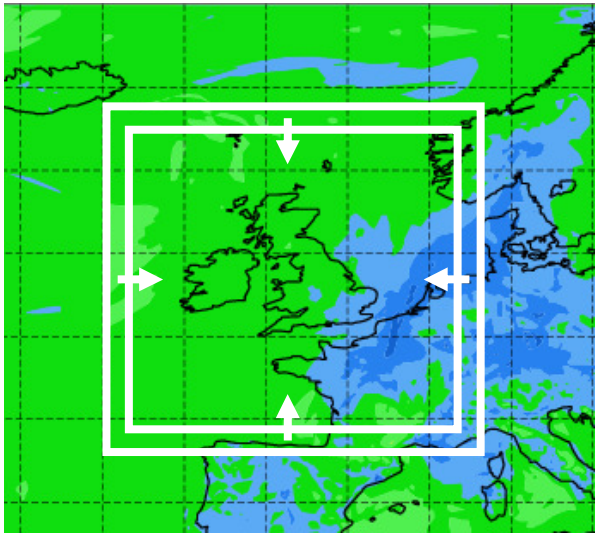
Air quality Modelling

Nick Savage, Paul Agnew, Lucy Davis, Carlos Ordonez, Marie Tilbee

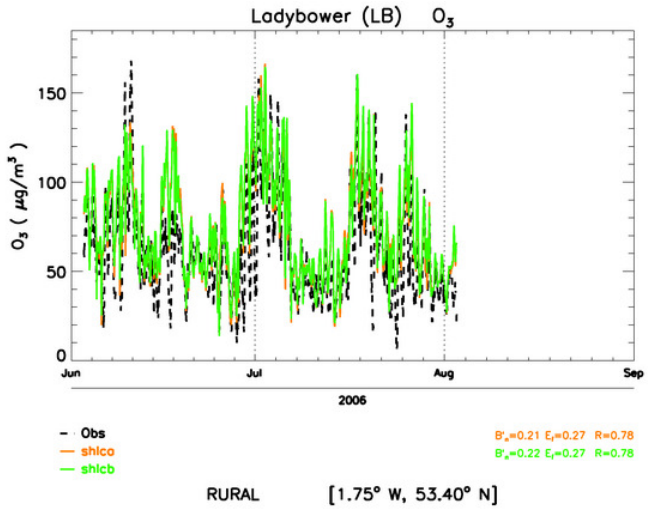
Air Quality in the Unified Model - AQUM

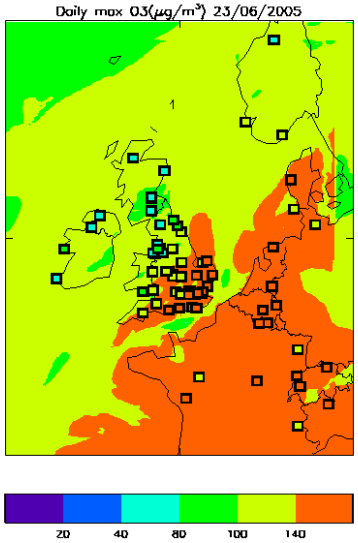
- Operational model, 5 day forecast, run daily
- Meteorological BC from Met Office Global model
- Chemical and aerosol BC from MACC-II real time forecasts
- Uses RAQ chemistry scheme, CLASSIC aerosol
- Post-processing includes bias correction using observations from the national monitoring network





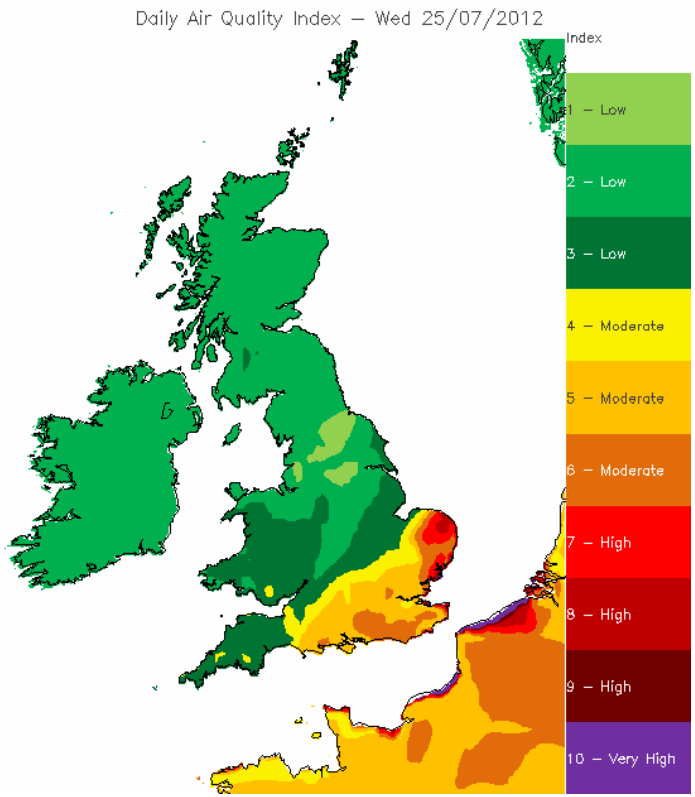
Near-real-time verification

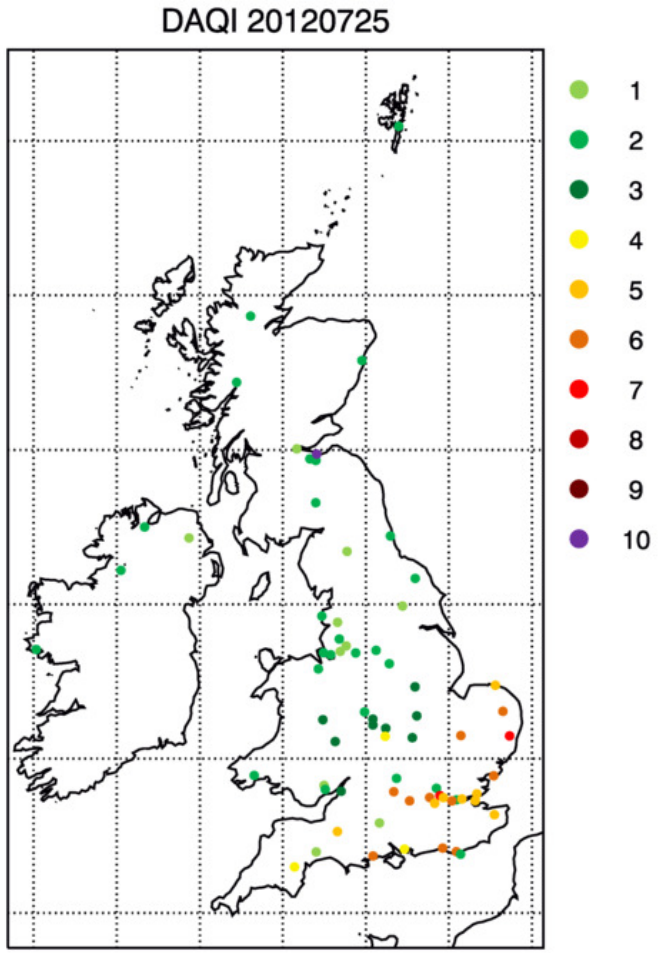




- We conduct routine verification against observations from the UK Automatic Urban and Rural Network (AURN)
  - Surface measurements of O3, NO2, NO, CO and PM are available
- This provides a rapid method of evaluating the forecast on a daily basis
- Constant objective evaluation aids our model development

Wednesday 25th July – week before Olympics opening ceremony





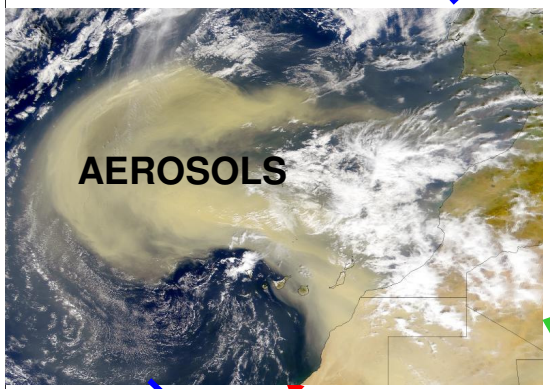
New Earth System Model

Fiona O’Connor

Radiation, cloud

Greenhouse Effect

Radiation & cloud through photolysis



Earth System Model

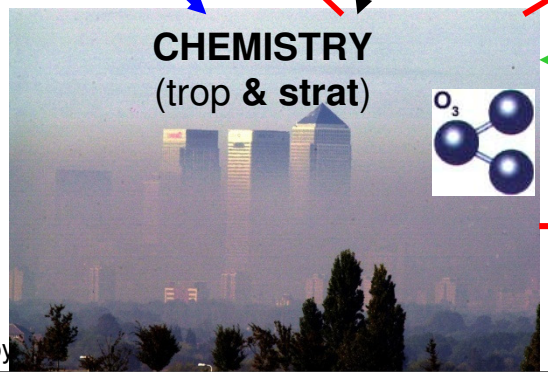
SO_4^{2-}, **NO_3^-, SOA formation**

DMS, dust, emissions

Heterogeneous chemistry, photolysis

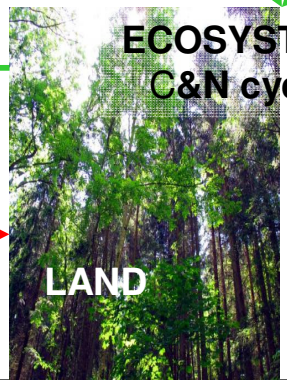
CO_2, **N_2O**

CH_4, **N_2O, CFCs**, trop & **strat** O_3



Wetland CH_4, dry dep, stomatal uptake, **BVOCs, N emissions**

O_3 damage, N Deposition



OCEAN (+shelf?)

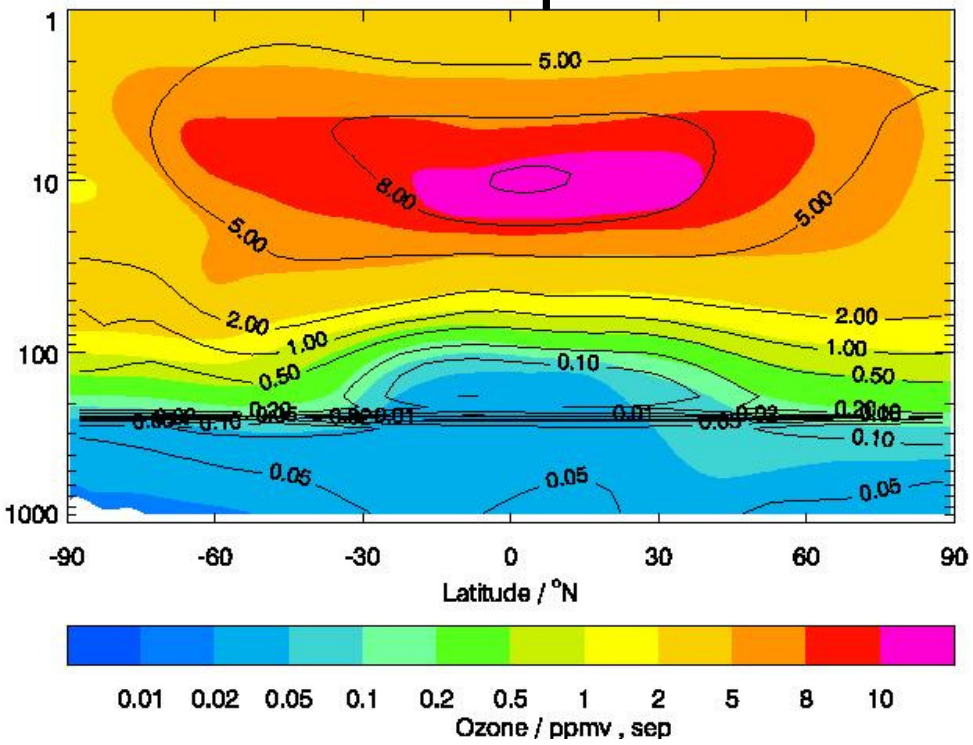
New Earth System Model UK-ESM1

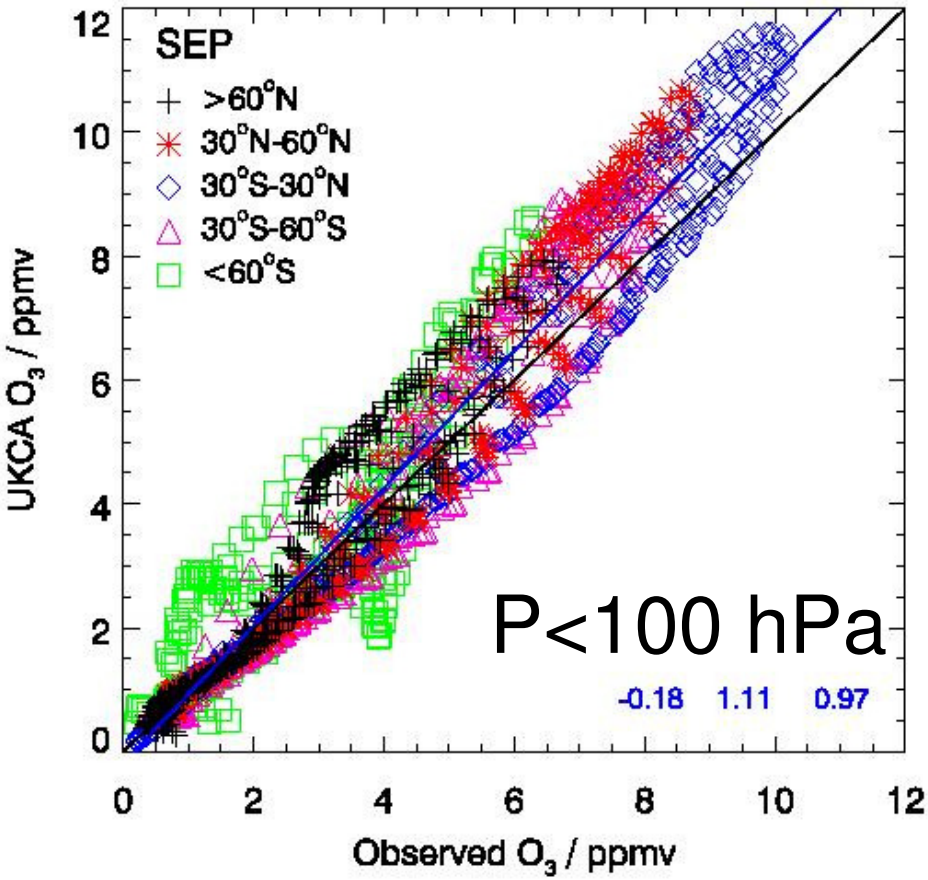
- Collaboration with NERC
- Whole atmosphere chemistry (stratosphere and troposphere)
- Interactive Biogenic VOC
- Fast-JX interactive photolysis scheme
- GLOMAP-mode aerosols (including nitrate and dust)
- Direct and indirect effects of aerosols

Progress so far (1)

Zonal mean ozone From Fiona O'Connor

Sep



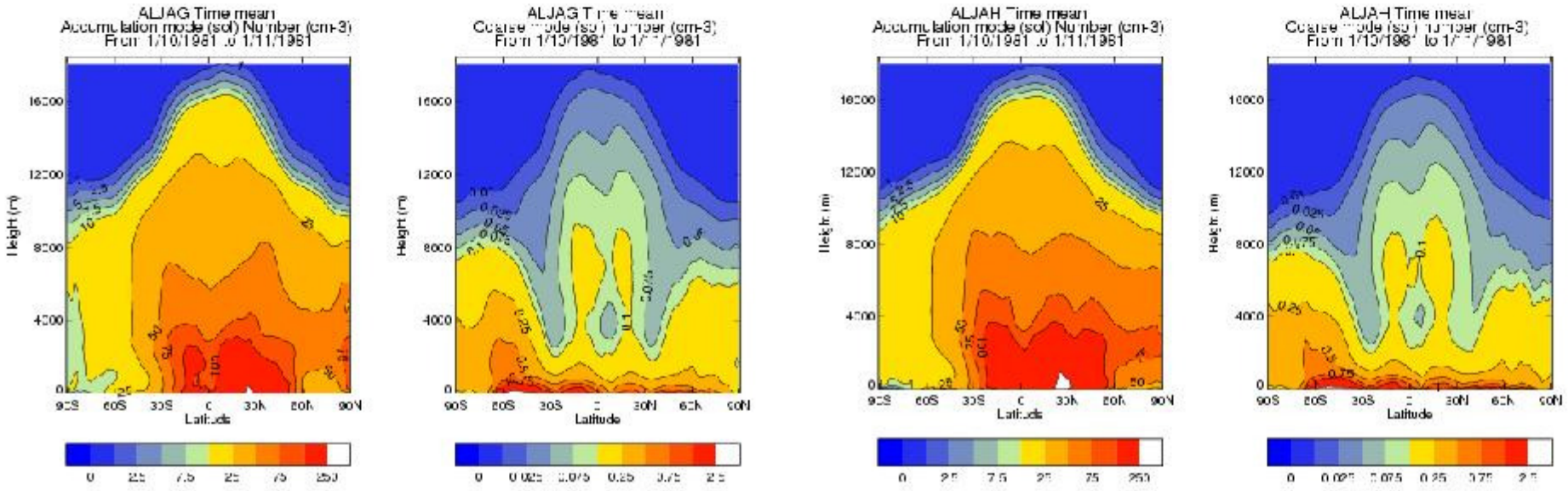


Model: UKCA (20-year monthly mean)
Obs: NIWA climatology (Hassler et al. 2009)

Progress so far (2)

MODE Aerosols with Offline Chemistry

From Colin Johnson



Online Chemistry Offline Chemistry

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

More information

More information

- Documentation paper UMDP 84 (on collaboration wiki)
- UKCA website: 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

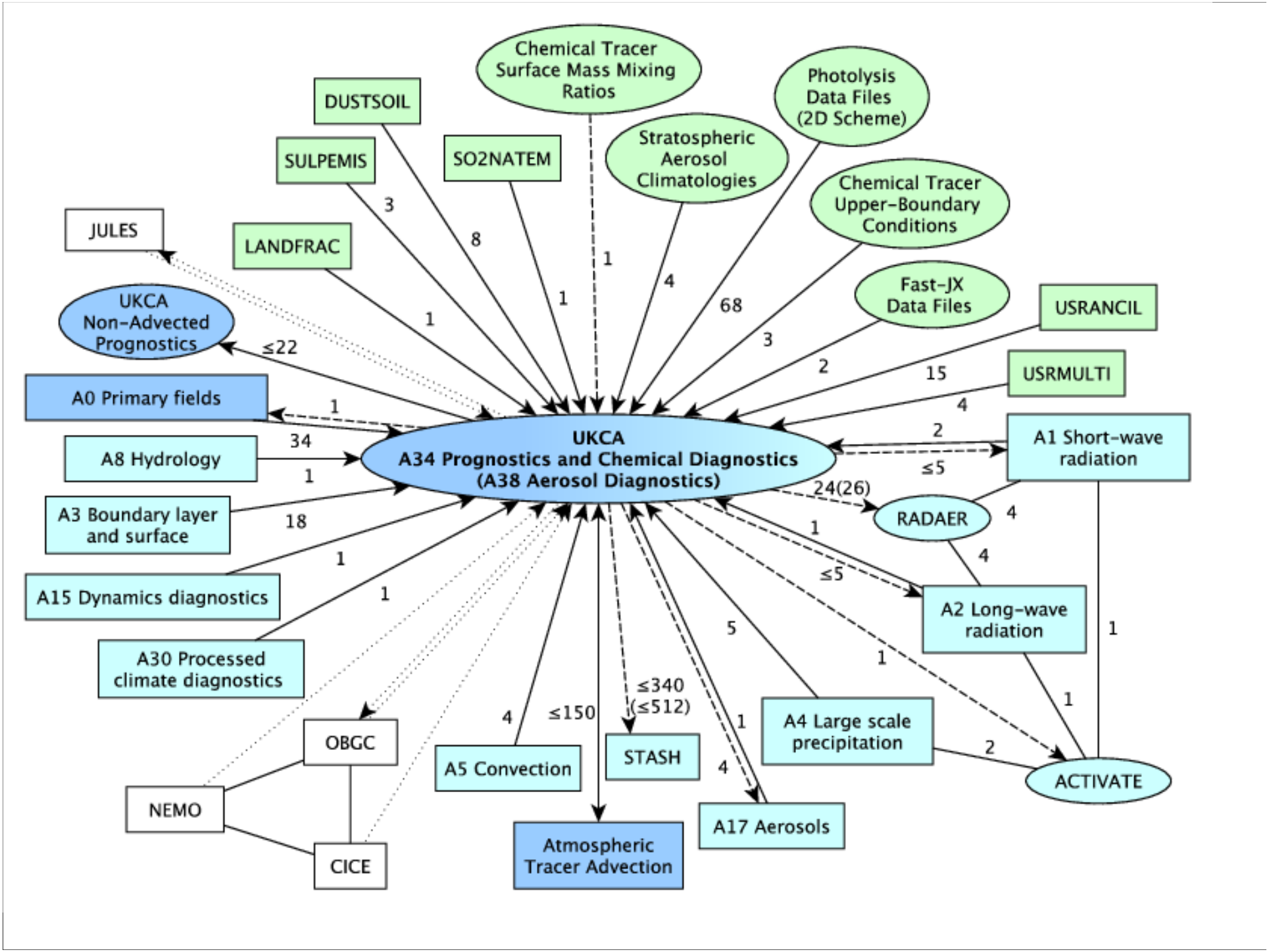
- At vn8.2 much of the NCAS community code lodged to the trunk
  - Required major effort to merge code at vn7.3 and then update to to vn8.1
  - Not sustainable process
- New aim is an approach where jobs shared between Met Office and partners are updated annually
- First jobs to be released soon (currently 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)


Chemical Tracer Surface Mass Mixing Ratios
Photolysis Data Files (2D Scheme)
DUSTSOIL
SULPEMIS
SO2NATEM
Stratospheric Aerosol Climatologies
Chemical Tracer Upper-Boundary Conditions
JULES
LANDFRAC
Fast-JX Data Files
USRANCIL
UKCA Non-Advected Prognostics
USRMULTI
A0 Primary fields
UKCA
A34 Prognostics and Chemical Diagnostics
(A38 Aerosol Diagnostics)
A1 Short-wave radiation
A8 Hydrology
A3 Boundary layer and surface
RADAER
A15 Dynamics diagnostics
A2 Long-wave radiation
A30 Processed climate diagnostics
A4 Large scale precipitation
OBGC
A5 Convection
STASH
ACTIVATE
NEMO
A17 Aerosols
CICE
Atmospheric Tracer Advection
3
8
1
1
4
68
3
2
15
4
≤22
1
34
1
18
1
1
2
≤5
24(26)
4
4
1
≤5
5
1
1
≤340
(≤512)
4
≤150
1
4
2
1