Report on Chemistry and Aerosols Modelling in UKCA

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1 Introduction

The development of Global Environment Models like the Hadley Centre model HadGEM2, with an explicit treatment of biospheric processes creates both requirement and opportunity to model the interactions between the biosphere, atmospheric chemistry, aerosols and climate processes. In addition, there is a need to continue to improve the modelling of aerosol processes in order to reduce the uncertainty in the forcing estimates (Houghton et al., 2001). These requirements establish the need for a new modelling approach for atmospheric chemistry and aerosols within the Climate Model, one which permits the interactions between the various model components, and that will lead to improved estimates of climate forcing.

This report covers work done in the development and appraisal of the U.K. Chemistry and Aerosols (UKCA) model. The UKCA model is being developed as a community model designed to be part of the Unified Model (UM) system. It is being developed such that chemistry-aerosol interactions can be easily included. UKCA is also being developed to enable both stratospheric and tropospheric chemistry to be treated in the same model. UKCA uses the UM semi-Lagrangian tracer transport scheme for the prognostic tracers. Work in the development of this model has been done in the following areas: tracer transport, tropospheric chemistry, stratospheric and combined stratospheric-tropospheric chemistry, aerosol chemistry, aerosols, and model interfaces.

The initial project partners are the Met Office (tropospheric chemistry, model interfaces, and aerosol chemistry), University of Cambridge (stratospheric and whole-atmosphere chemistry), and University of Leeds (aerosol microphysics). Other organisations are also becoming involved, and UKCA is already being used as a research tool. Further details of UKCA are being made available on a web site (http:\\www.ukca.ac.uk).

2 Objectives of UKCA

The UKCA project was set up to provide a new framework for atmospheric chemistry and aerosols within the climate model. This was in response to a situation where the modelling effort in these areas was carried in seperate models making communication difficult and model maintainence too costly. Two main target areas were selected: a combined stratospheric-tropospheric chemistry model, and a combined chemistry-aerosols model. The combined stratospheric-tropospheric chemistry model is required so that interactions between ozone recovery in the stratosphere, ozone growth in the troposphere and climate change can be adequately simulated. The chemistry-aerosols model will provide an improved aerosols model combined with the ability to include chemistry-aerosols interactions. It is important to include these interactions as they affect both the chemistry and the aerosol concentrations (Liao et al, 2003). Table 1 shows the main chemical and aerosol schemes which are being tested as components of UKCA, together with the number of transported tracers required and the main emitted species.

3 Tracer transport tests

The UKCA model is being developed using the atmosphere model HadGAM1 at a resolution of 3.75° × 2.5° with 38 levels for tropospheric chemistry and with sixty levels for stratopheric chemistry. It is also being tested using models at a resolution of 1.875° × 1.25° . In order to assess the tracer transport scheme and to highlight any resolution dependence, work on testing the tracer transport scheme with a variety of idealised tracers has been done.

3.1 Radon

In this experiment, radon (Rn-222) was emitted from all non-frozen land points, followed by radioactive decay to lead (Pb-210) with a half life of 3.8 days. This tracer is useful as it highlights short-term atmospheric transport processes such as convective transport and boundary-layer mixing. In some experiments, the lead was retained as a neutral tracer so that the sum of the radon and lead in the model should equal the accumulated radon emissions. This tests the mass conservation of tracer transport scheme and was found to be satisfactory at all resolutions.

Figure 1 shows the comparison between simulated and observed (Genthon and Armengaud (1995), Dentener et al. (1999) and Hauglustaine at al. (2004)) radon concentrations at the surface for selected stations. The comparison shows satisfactory agreement for most sites, however the simulation at some sites such as Bombay shows differences which are likely to be attributable to differences between model circulation and the circulation at the time of the observation. Figure 2 shows the comparison between observed (Kritz et al., 1988) and simulated profiles of radon near San Francisco (Moffet Field, 37.4° N, 122.0° W). All modelled profiles capture the steep vertical gradient in the boundary layer but only output from June appears to capture the enhanced concentrations in the upper troposphere, however seven out of the eleven flights were in June.

3.2 Lead

The isotope Pb-210 is a product of the radon decay sequence, and we have simulated this product by treating it as a species attached to fine aerosol. This tracer will therefore respond to dry and wet deposition processes in the model. Figure 3 shows the comparison between simulated and measured surface concentrations of Pb-210. The measured surface concentrations were taken from SASP (2005). In general, the annual cycle of the measurements is followed quite well by the model results. In addition the model deposited lead also correlates quite well with measured values (Priess and Grenthon, 1997).

3.3 Krypton

The isotope Kr-85 is emitted during reprocessing of nuclear fuel. In this experiment, krypton was emitted from seven known point sources in the northern hemisphere during the period 1978-1983. The strength of these sources was taken from Jacob et al. 1987. Krypton was also emitted from a nuclear reprocessing plant in the former USSR, whose strength was estimated by Jacob et al. 1987. The experiment was done using both N48 (3.75° × 2.5°) and N96 (1.875° × 1.25°) resolutions, Fig. 4 shows that the dispersion in the model was similar at both resolutions. The modelled results can be verified by comparison with observations (Jacob et al., 1987). Nine observed meridional profiles of krypton were obtained during ship cruises over the Atlantic Ocean between 1980 and 1987. The comparison for March (Fig. 5) clearly shows that there is a strong difference between the model years and that the results for March 1983 will be sensitive to the model initialisation which was taken from Rind and Lerner (1996). However, the meridional gradient seems quite robust in all model years and occurs at approximately 0N. This matches quite well with the observed tropical gradient. From the interhemispheric gradient and the mean emission rate, the timescale for interhemispheric transport may be estimated, this was 1.33 years at the N48 resolution and 1.3 years at N96.

4 Tropospheric chemistry

A tropospheric chemistry scheme involving 24 tracers, 27 photolysis reactions and 101 gas-phase reactions has been included in UKCA. The chemistry involves the oxidation of methane, ethane and propane, with an optional isoprene degradation scheme developed at the University of Cambridge. The model does not yet have a reresentation of heterogenous reactions. Surface, lightning, and aircraft emissions are included and processes such as dry deposition, convective and large-scale washout are also considered. As this scheme lacks stratospheric chemistry, boundary conditions are required at the top of the model domain. For ozone, all levels above 30 hPa are set to values taken from a climatology derived from the Cambridge two-dimensional model.

Figure 6 shows surface carbon monoxide concentrations compared with observations at selected sites for a multi-annual simulation of HadGAM with UKCA. Concentrations in the southern hemisphere are too high, probably indicating incorrect emissions here, but the seasonal cycle is correct at most sites, particularly the subtropical ones. Figure 7 shows the simulated surface ozone concentrations compared to observations. The model simulates the springtime ozone maxima at northern hemisphere sites, though this persists for too long. The seasonal cycles at Mauna Loa and Bermuda closely match the observations, but the summertime ozone concentrations are too high at Cape Grim. This is possibly because both carbon monoxide and methane concentrations are also too high here.

Figure 8 shows modelled and measured ozone profiles for a selection of sites for July. The measurements are taken from the analysis of Logan (1999). The simulated profiles have similar shapes to the observations, though there are considerable differences shown at some sites, notably an overprediction at Alert. Other analysis of the ozone profiles shows that that model errors in tropopause height are a source of error at some sites.

As well as the standard chemistry scheme described above the chemistry of isoprene degradation has been added to the model using a condensed mechanism based on the Mainz scheme (Pöschl et al., 2000) with twelve additional tracers and two steady-state species. The emissions of isoprene were taken as being 500 Tg/yr as [C], and the carbon monoxide emissions in the model were adjusted to take out the component added when isoprene is not included. Figure 9 shows modelled and measured (Emmons et al., 2000) profiles of O_3 , CO , HNO_3 , PAN , NO_x , C_3H_6 , and C_3H_8 for Hawaii. The model with the isoprene mechanism shows considerably more CO and PAN than the simple mechanism. The increases to C_3H_6 and C_3H_8 show that there has been a reduction in the oxidation of these species by OH, and this change will have also impacted on the CO. Both simulations show too much nitric acid, but the simulation with isoprene shows a large increase in PAN. This feature is shown in other modelling studies.

5 Stratospheric Chemistry

Stratospheric processes are included in the remit of UKCA, as discussed before, to provide a platform to study climate change in the stratosphere, its coupling with and impact on tropospheric processes, and its response to anthropogenic and natural forcings, for example, the release of halogens from industrial processes and volcanic eruptions. Basically, the whole-atmosphere version of UKCA is largely identical to the tropospheric version but has some additional features which may be disactivated for tropospheric chemistry. Mainly, the gas phase chemistry is extended to include stratospheric halogens (chlorine and bromine) and their source gases, nitrous oxide as a source of NO_x, some additional shortlived radicals, a number of additional reactions usually neglected in tropospheric chemistry, and heterogeneous chemistry on polar stratospheric clouds, tropospheric ice and sulphate aerosol. For photolysis, an online formulation of photolysis rates has recently been included that comprises the UV wavelengths of relevance in the stratosphere (down to 175 nm wavelength) and accounts for absorption and scattering due to clouds, aerosols and gas phase molecules throughout the entire column. It optionally replaces somewhat cheaper off-line photolysis rates interpolated from two different tables, one used in the troposphere, as discussed before, and one with different parameters for middle-atmospheric processes. This off-line approach is also always used in the mesosphere where the online formulation is not applicable. For heterogeneous chemistry, a basic formulation is adopted that accounts for the reactions that transform reservoir chlorine (HCl, $ClONO_2$) into active chlorine (HOCl, ClO_x) and also converts N_2O_5 to $HONO_2$, especially after volcanic eruptions. Almost all of the simulations done so far were with chemical families (O_x, NO_x, ClO_x, BrO_x). However, recently a non-families Newton-Raphson solver has been added which is expected to produce more accurate results. The simulation discussed below is with the families approach; short runs with the non-families solver have been used to identify the reason for certain problems with the families approach.

Figure 10 shows the mean annual ozone column as derived from a ten-year integration. In most of the domain, the correspondence with climatology (derived from the TOMS/SBUV data) is quite good. In the tropics, an underestimation of the ozone column by about 20 DU may be due to insufficient tropospheric ozone production due to non-representation of organic ozone precursors. Over the South Pole, the ozone column in the climatology is substantially smaller than in the model. Figure 11 shows the zonal-mean ozone distribution in January and July, juxtaposed to the UARS/HALOE climatology. Again, in much of the domain the correspondence is good, except over the poles and higher up in the atmosphere. This problem is not apparent in a simulation with the non-families solver.

Figure 12 shows zonal a typical mean odd nitrogen ($NO + NO_2 + HNO_3$) cross section versus the UARS climatology. Substantial differences appear, especially at high latitudes. The odd nitrogen content of the stratosphere is very sensitive to transport and temperature and hence provides of better measure of model performance than ozone. The excessively depleted air over the winter pole correlates with very low values of CH_4 , for example, and indicates that the air is largely of mesospheric origin. This issue seems to be connected to a model dynamics problem giving too strong descent over the poles (see below).

Figure 13 shows zonal-mean ClO. Here, the model again systematically underpredicts the amount of ClO to be expected. Again, the non-families solver is expected to perform better on this but a definitive statement requires a longer run than is available so far.

Figure 14 shows the zonal mean temperature differences with respect to the SPARC temperature reference. In the middle stratosphere positive biases occur, peaking over the poles at around 8 K. The positive bias explains why chlorine activation is insufficient to create realistic ozone depletion in the southern polar vortex. This problem is being addressed in a more recent version of the background L60 model with improved temperature structure. The erroneous temperature structure is also linked to transport anomalies. To assess this problem, a tracer transport intercomparison was performed, using the available stratospheric models (UKCA, UM 6.1 L60, UM 4.5 L64, and SLIMCAT). A mesospheric tracer was set to 1 above 1 hPa, and left unchanged elsewhere. Figure 15 shows the mixing ratio of this tracer in October, after 13 months of integration. The UKCA model (based on an older version of the L60 model) transports the mesospheric tracer to lower altitudes than the "Old Dynamics" UM 4.5 model and the off-line transport model SLIMCAT, driven with UKMO analyses. This finding is consistent with the low odd nitrogen found there. A similar integration with improved radiation (Wenyi Zhong mods) yields a somewhat improved temperature in the middle stratosphere, but early indications are that the temperatures over the winter pole are still too high and downward transport from the mesosphere too strong, compared to observations and the "Old Dynamics" model (which, driven with similar chemistry, produces more realistic total nitrogen).

In summary, due to recent inclusions of a more sophisticated photolysis scheme, heterogeneous processes on sulphate aerosol, and a newly incorporated non-families solver, the stratospheric chemistry component of UKCA is now in substantially better shape than before. On the dynamics front, changes to the radiation scheme have made a significant improvement in temperature. However, further tuning may still be necessary to improve transport in the Middle Atmosphere. At present, we are in the process of assessing exactly which effect the improved dynamics will have on chemistry, and vice versa.

6 Aerosol Scheme

The multi-component multi-modal UKCA aerosol scheme has been named "UKCA-mode" and advects both the particle number and component masses in a number of internally mixed modes (i.e. it is a two-moment scheme). This enables an improved representation of aerosol microphysical processes (e.g. H_2SO_4 vapour condensation, coagulation and in-cloud oxidation). These processes control the evolution of the size distribution, composition and mixing state of the aerosol population and hence determine their optical properties and role in climate forcing.

Two formulations of the scheme are in development — a "standard" 7-mode scheme with four water-soluble and three water-insoluble modes and a "reduced" scheme with just the four soluble modes. New particles are generated in the model from binary H_2SO_4 - H_2O nucleation (following Kulmala et al, 2000) and primary emissions.

The aerosol components included in UKCA-mode are sulfate, ammonium, nitrate, sea-salt, black carbon, organic carbon, dust, sea-salt and water. The 7 internally mixed modes in the standard version enable the ageing of initially insoluble aerosol (e.g. dust, black carbon) to become soluble at a rate detemined by their rate of coagulation with soluble particles and the rate of condensation of H_2SO_4 onto them.

The standard and reduced UKCA aerosol schemes will require 25 and 18 tracers to be advected respectively (cf 15 in the current UM scheme). The equations for the micro-physics are solved process- split with analytical solutions. The tracer advection will likely be the limit for computational speed.

6.1 Status and Progress

The UKCA aerosol scheme is being developed and tested within the offline chemistry transport model TOMCAT. The version of the CTM currently being used incorporates a 7-species sulfur chemistry scheme (DMS, SO_2 , H_2SO_4 , DMSO, MSA, COS, CS_2) and currently has the standard TOMCAT chemistry switched off with oxidants O_3 , OH , NO_3 , H_2O_2 and HO_2 provided via interpolations between six-hour monthly mean fields from a "full chemistry" TOMCAT run.

The current version of UKCA-mode being tested and evaluated includes sulfate, sea-salt, black carbon (BC), organic carbon (OC) and water with dust, nitrate and ammonium to be added in the next few months. Aerosol and precursor emissions match those in the AEROCOM project (Kinne et al., 2005) to facilitate evaluation against observations. Their sources are both natural (e.g. oceanic DMS and sea-salt, volcanic SO_2 and sulfate) and anthropogenic (e.g. SO2 and sulfate from industry, power-plants, transport and domestic sources, SO2, sulfate and BC/OC from vegetation fires and BC/OC from bio-fuel and fossil-fuel sources).

Figure 16 shows a global map of monthly mean column mass concentrations of sulfate, black carbon, organic carbon and sea-salt for a T42L31 resolution UKCA-TOMCAT run for June (using 1996 meteorology). Figure 17 shows a zonal mean plot of particle number and mean particle size in the nucleation mode highlighting the variation in size of the particles. Figure 18 shows a global map of the burden, mass flux and ageing rate of black carbon aerosol particles at the surface.

The aerosol scheme will be implemented into the UM over summer 2006 and testing/evaluation of the complete UKCA-UM (chemistry + aerosols) will proceed from the autumn. The UM radiation scheme has also been updated to handle the internally mixed modes that UKCA generates.

7 Conclusions

The UKCA model is operating within the atmosphere model in a number of different configurations, and has been tested in a variety of different ways. For the tropospheric chemistry configuration, these include tests of the tracer transport with idealised tracers, and validation of chemical models against measurements of carbon monoxide, methane and ozone. UKCA is being included as part of the UM system, and as such will be available for use throughout the atmospheric modelling community in the UK. The Stratospheric chemistry configuration is being developed in parallel with the sixty level version of HadGAM at N48 and N96 resolutions. The climatology of this model has been improved with modifications to the long-wave ozone and CO_2 absorption and with improvements to the ozone climatology which was found to be unrealistically high in the lower stratosphere.

Remaining tasks to be done include porting and testing the aerosol scheme (UKCA-MODE) to the rest of UKCA, and solving remaining problems with the stratospheric component. Work in progress and not reported here includes the optimisation and porting of the FAST-J (Wild et al, 2000) photolysis model as an on-line component. Work to simplify the equilibrium chemistry involved in the calculation of aerosol internal mixtures is planned to commence as part of the QUEST (QUAAC) project, supported by projects at the Universities of Leeds and East Anglia. Work to provide estimates of the natural emissions of methane, isoprene, terpenes, and other species has been done at the Met Office and is also being developed in the QUEST project.

8 Acknowledgements

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9 References

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10 Tables

Scheme	Main Emitted Species	No of Tracers
1. Standard Tropospheric	NO_x , CH_4 , CO, C_2H_6 , C_3H_8	24
2. Extended Tropospheric	As 1, with Isoprene	36
3. Standard Stratospheric	As 1	15
4. Extended Stratospheric	As 3, with CFCs and N_2O	22
5. Aerosol Chemistry	SO_2 , DMS, NH_3	5
6. UKCA-MODE ”standard”	BC, OC, SS, DU	25
7. UKCA-MODE ”reduced”	BC, OC, SS, DU	18

Table 1: Chemical and aerosol schemes in UKCA. The standard stratospheric chemistry scheme is currently being tested using lower boundary conditions for species such as nitrous oxide, and the halogens.

Mode Name	Size Range (nm)	Composition	Soluble ?
Nucleation-sol	$\bar{r} < 5$	SU	Yes
Aitken-sol	$5 < \bar{r} < 50$	SU, BC, OC	Yes
Accumulation-sol	$50 < \bar{r} < 500$	SU, BC, OC, SS, DU	Yes
Coarse-sol	$\bar{r} > 500$	SU, BC, OC, SS, DU	Yes
Aitken-insol	$5 < \bar{r} < 50$	BC, OC	No
Accumulation-insol	$50 < \bar{r} < 500$	DU	No
Coarse-insol	$\bar{r} > 500$	DU	No

Table 2: Initial configuration for UKCA-MODE, based on the M7 model concept. Abbreviations for individual aerosol components are as follows: SU = sulphate, BC = black carbon, OC = organic carbon, SS = seas salt, DU = dust.

11 Figures

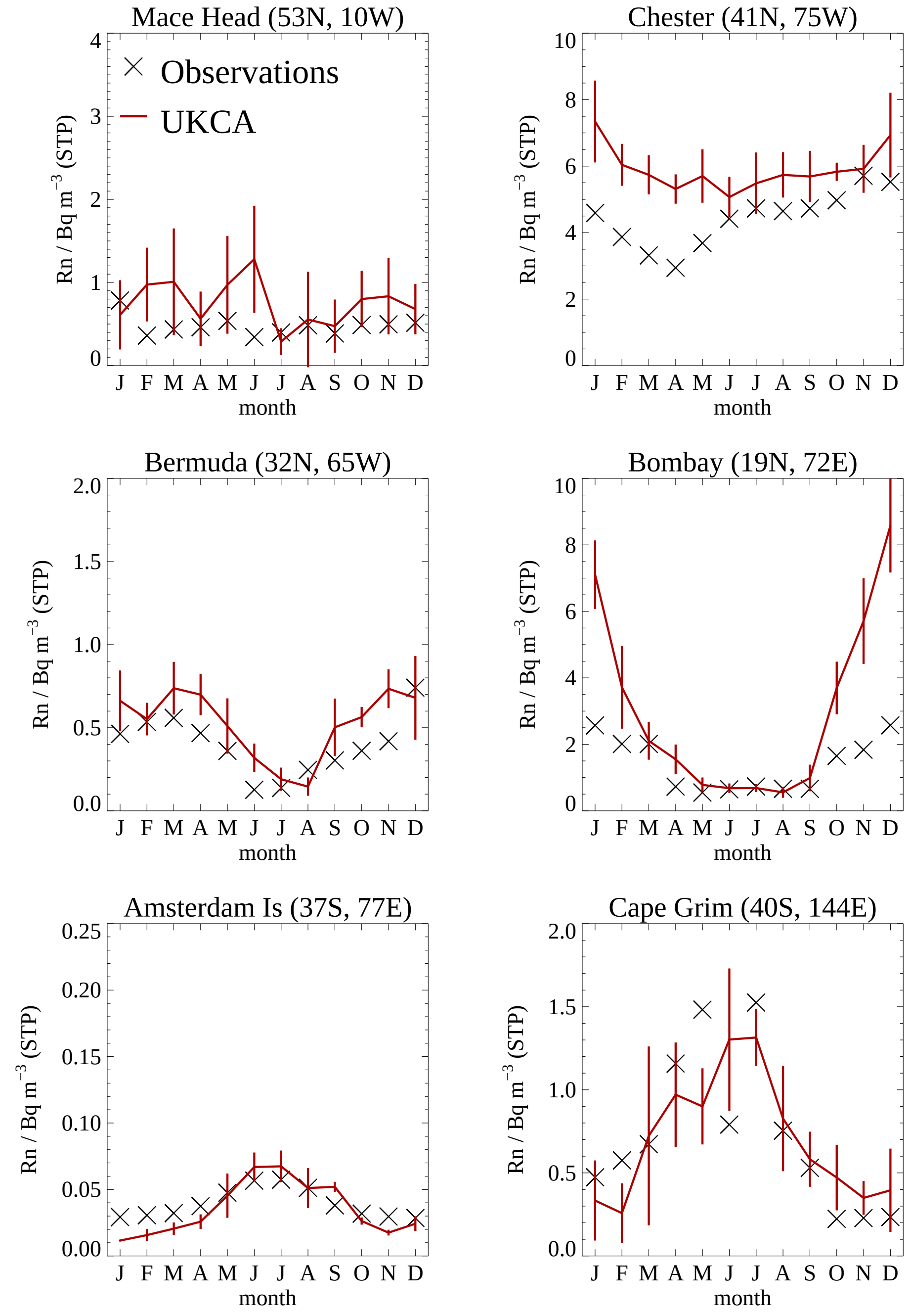


Figure 1: Surface concentrations of Radon-222 for a selection of sites.

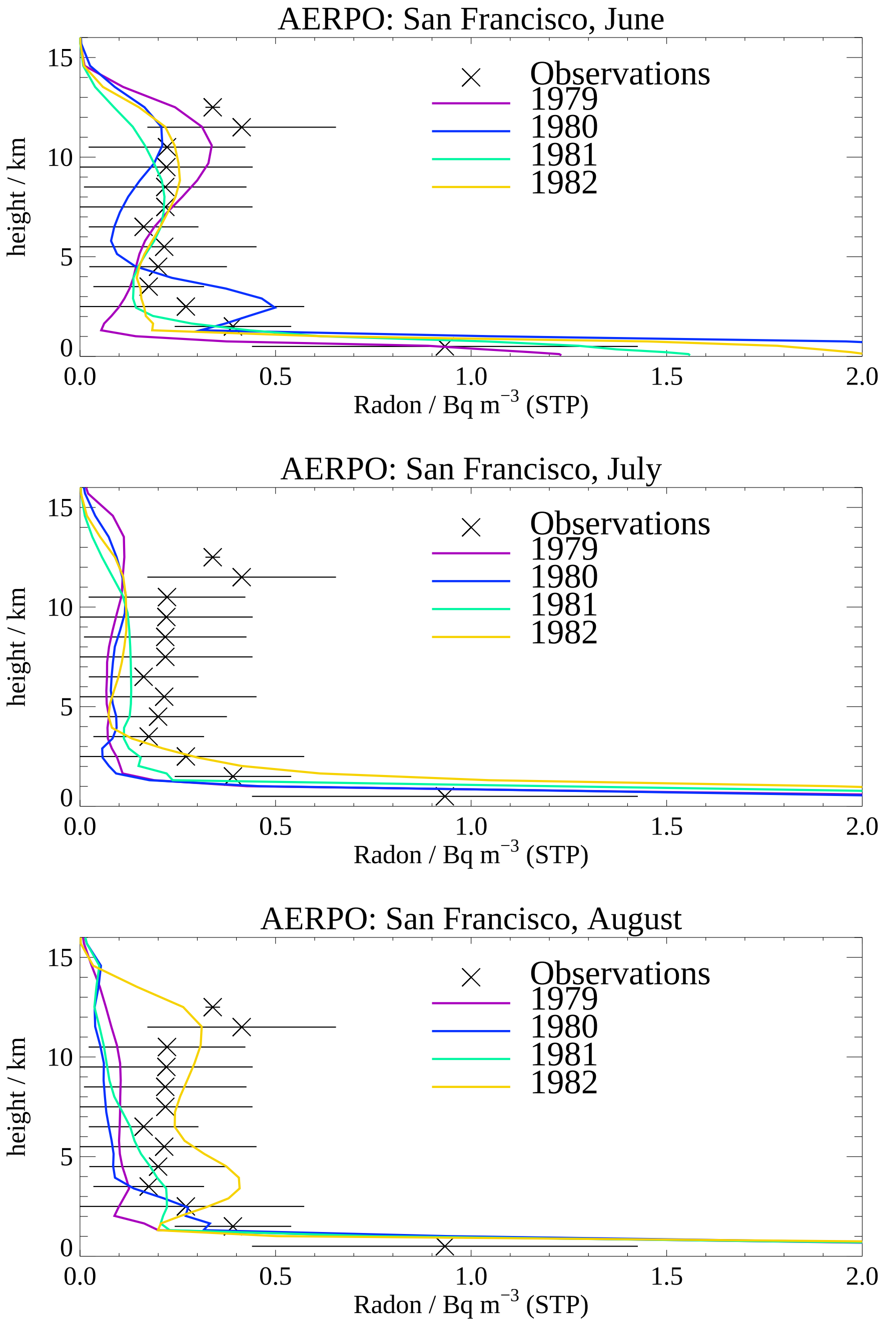


Figure 2: Modelled and measured profiles of radon-222 concentrations at San Francisco. The model results are shown for different years of the simulation.

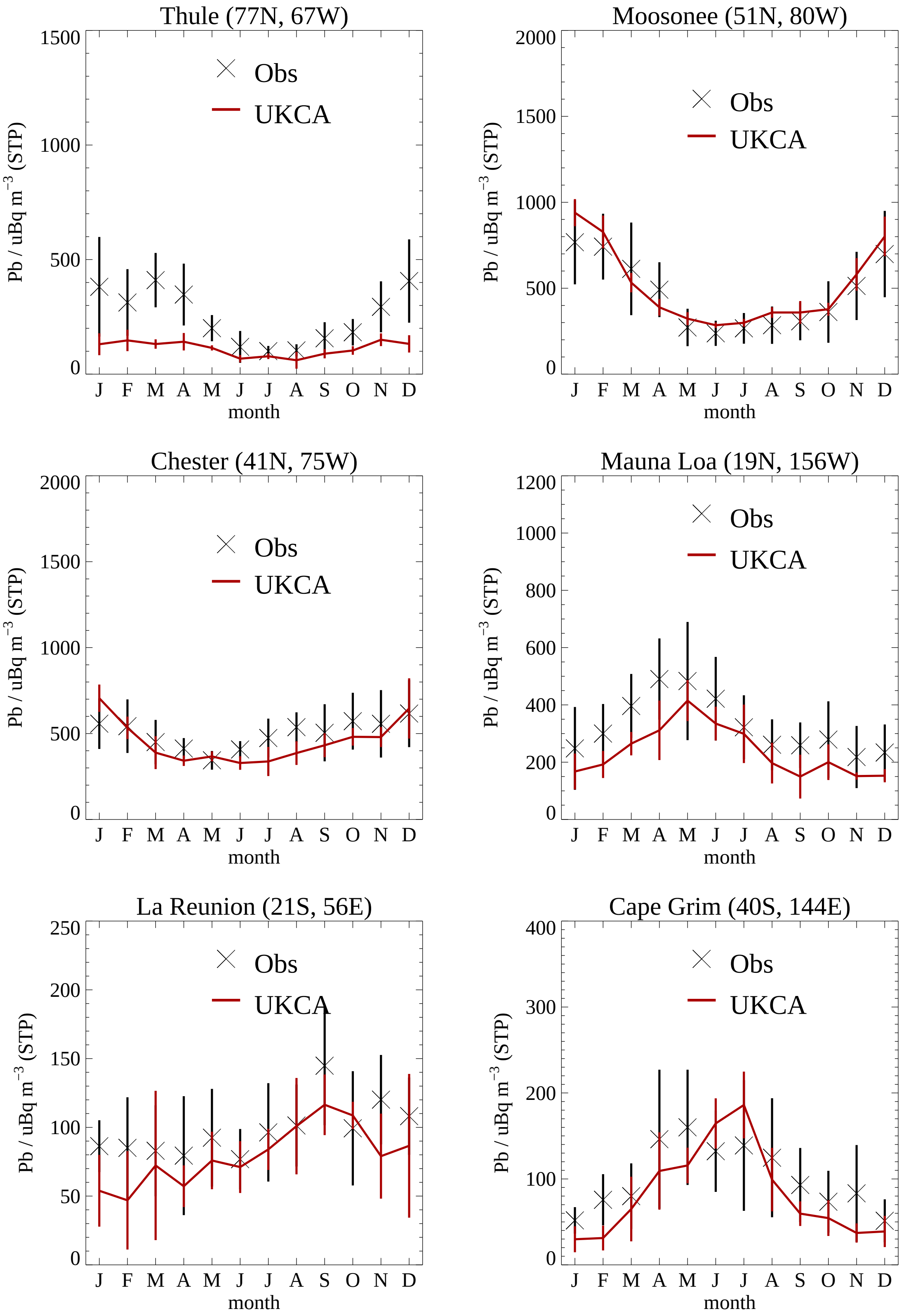


Figure 3: Surface Lead-210 concentrations simulated in UKCA compared to observations.

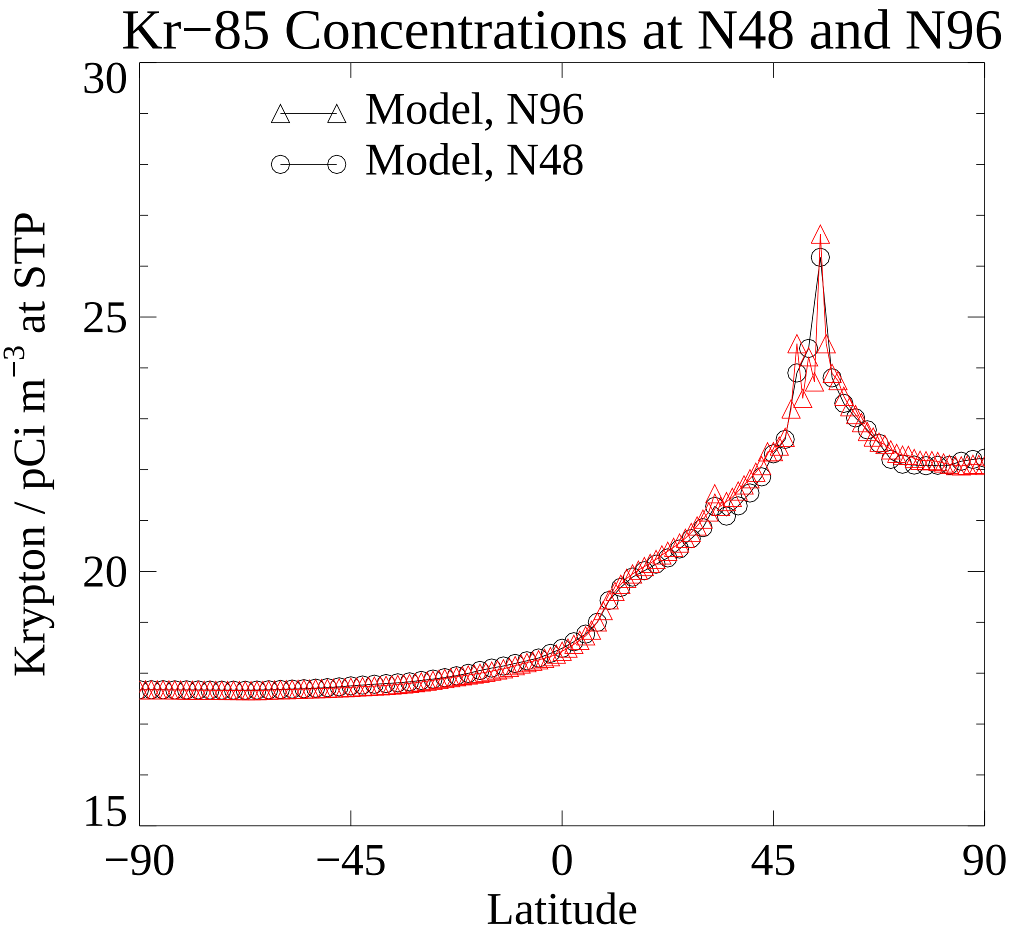


Figure 4: Surface Krypton-85 concentrations simulated in UKCA using N48 and N96 resolutions of the HadGAm1 model.

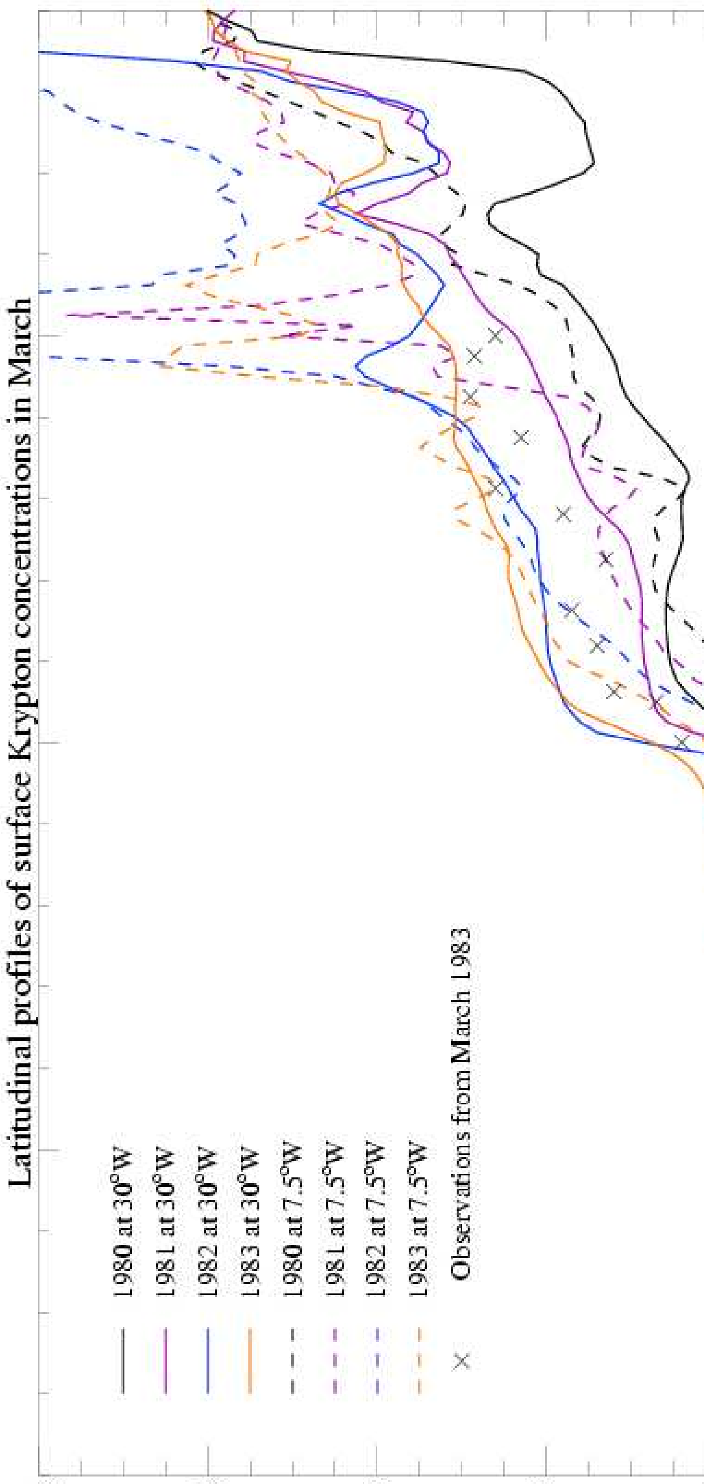


Figure 5: Surface Krypton-85 concentrations simulated in UKCA using the HadGAm1 model compared to observations.

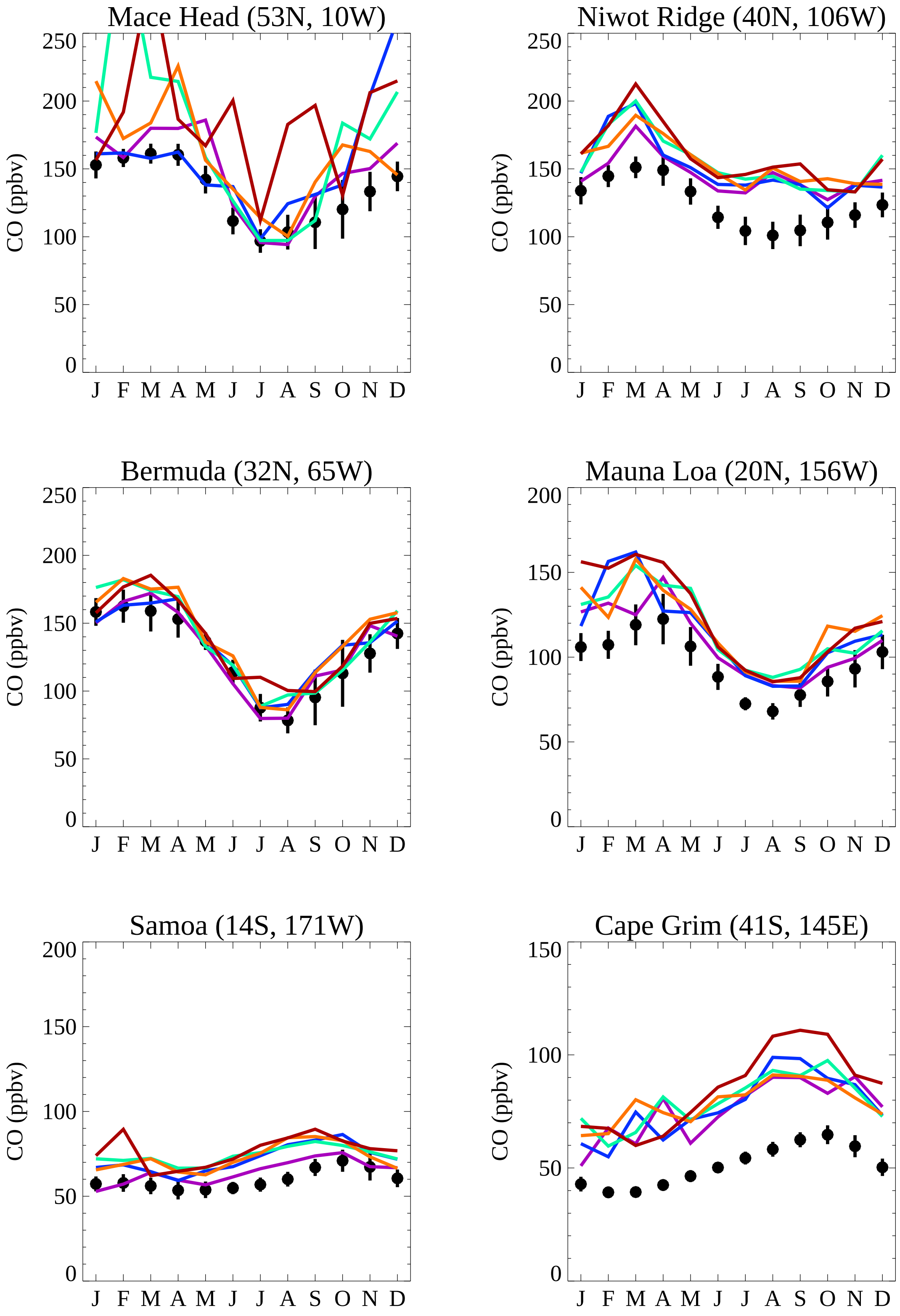
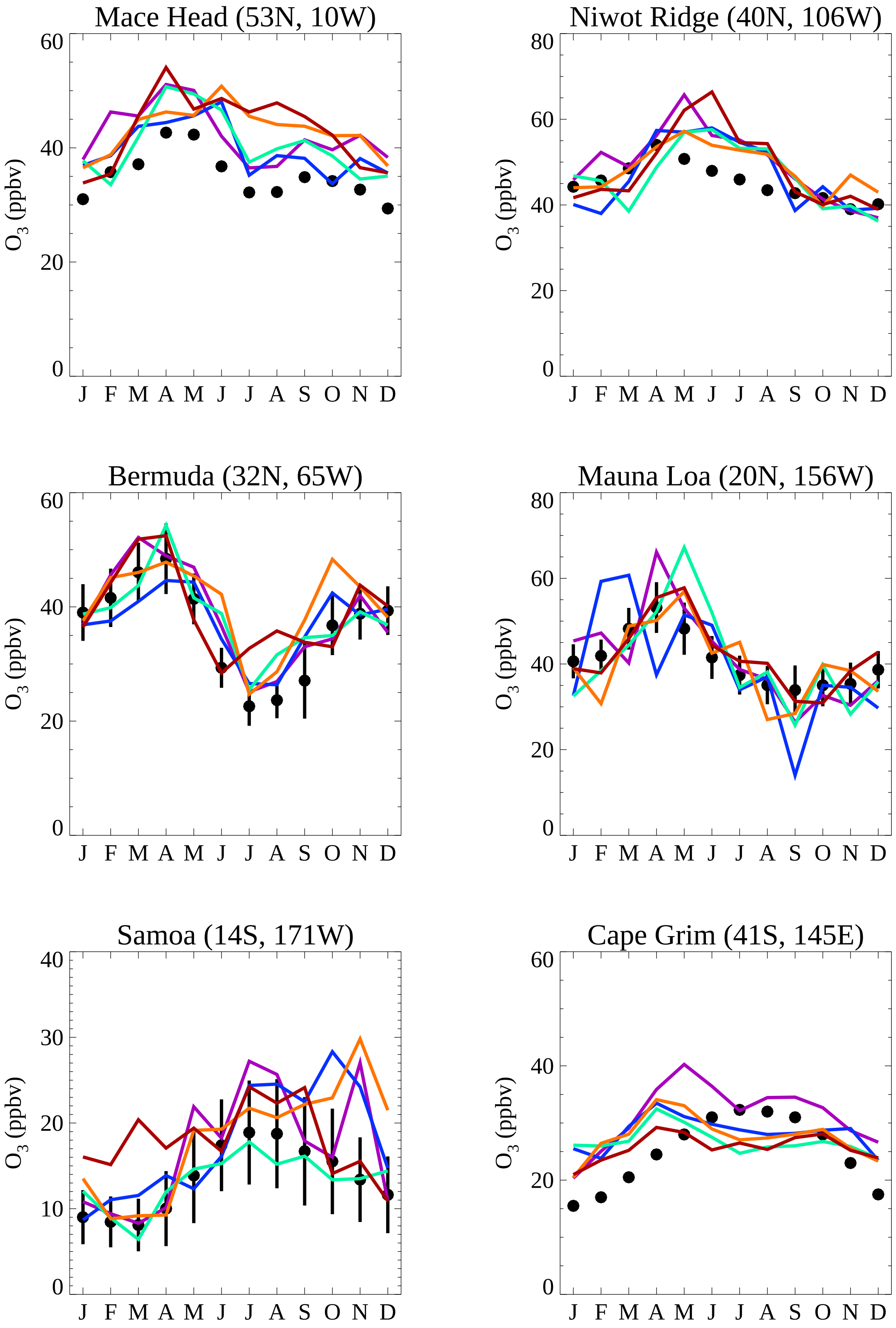


Figure 6: Comparison between simulated and observed surface carbon monoxide concentrations for selected sites. The lines represent different years of a five-year model run. Observations are taken from the CMDL network (CMDL, 2005).


Mace Head (53N, 10W)

Niwot Ridge (40N, 106W)

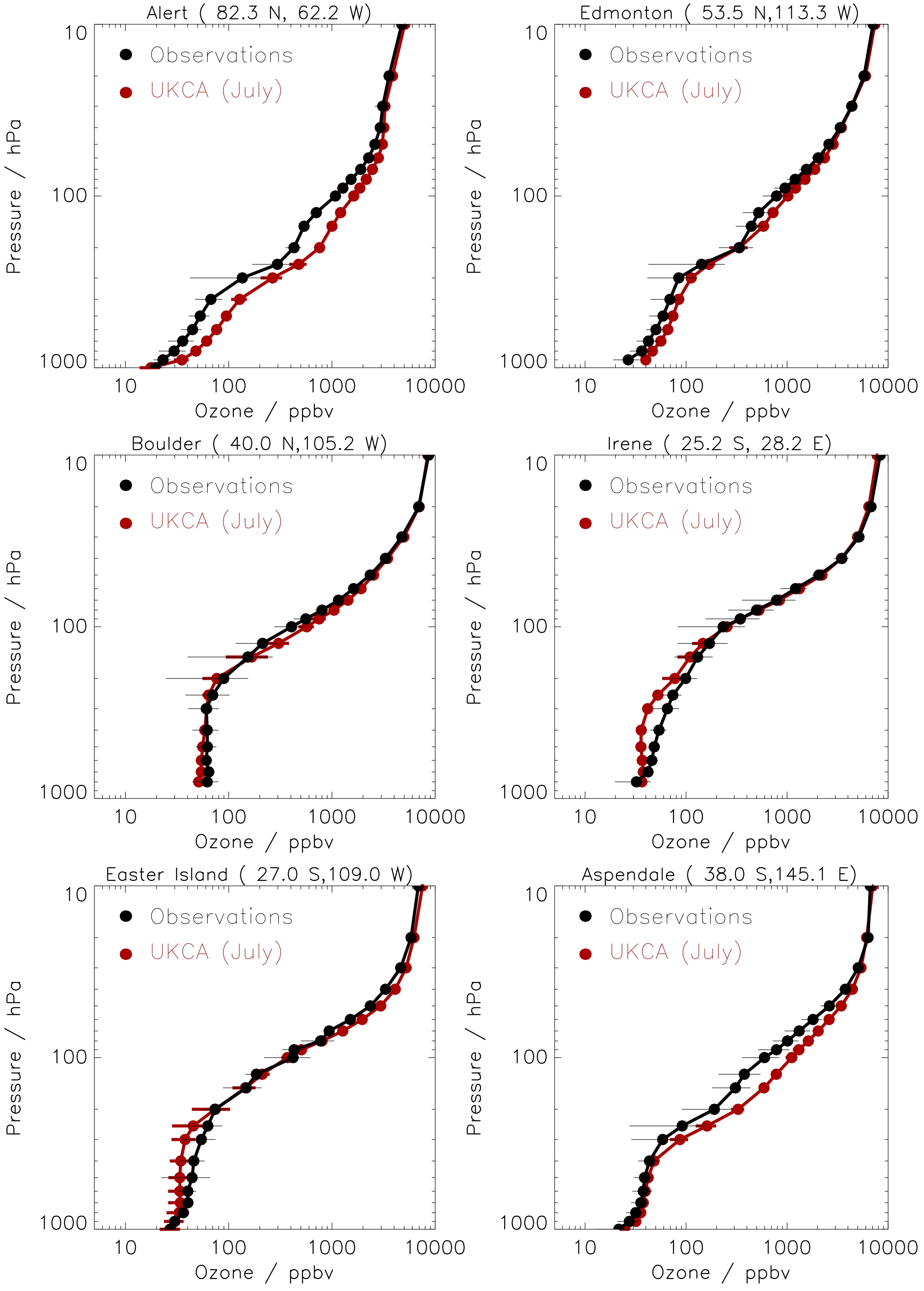
Bermuda (32N, 65W)

Mauna Loa (20N, 156W)

Samoa (14S, 171W)

Cape Grim (41S, 145E)

Figure 7: Comparison between simulated and observed surface ozone concentrations for selected sites. The lines represent different years of a five-year model run. Observations are from Oltmans and Levy (1994) and from CMDL (2005).


Alert (82.3 N, 62.2 W)

Edmonton (53.5 N,113.3 W)

Boulder (40.0 N,105.2 W)

Irene (25.2 S, 28.2 E)

Easter Island (27.0 S,109.0 W)

Aspendale (38.0 S,145.1 E)

Figure 8: Comparison between model ozone profiles with ozonesonde measurements (Logan et al., 1999). The model results are a mean of a five-year simulation.

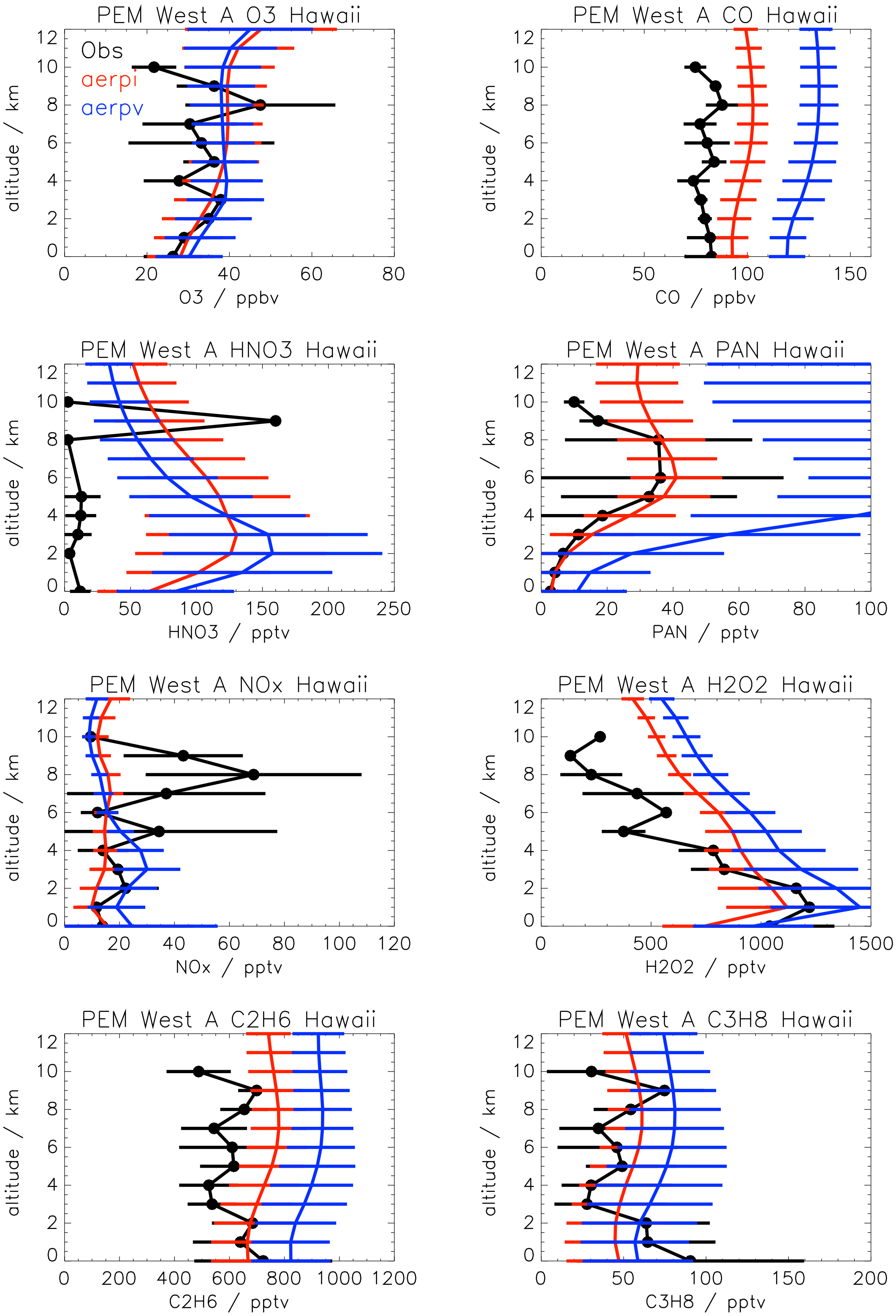


Figure 9: Comparison between measured and simulated profiles with measurements (Emmons et al., 2000) for Hawaii. The model results are a mean of a five-year simulation. Observations are in black, with results from simulations with (blue) and without (red) the isoprene mechanism included.

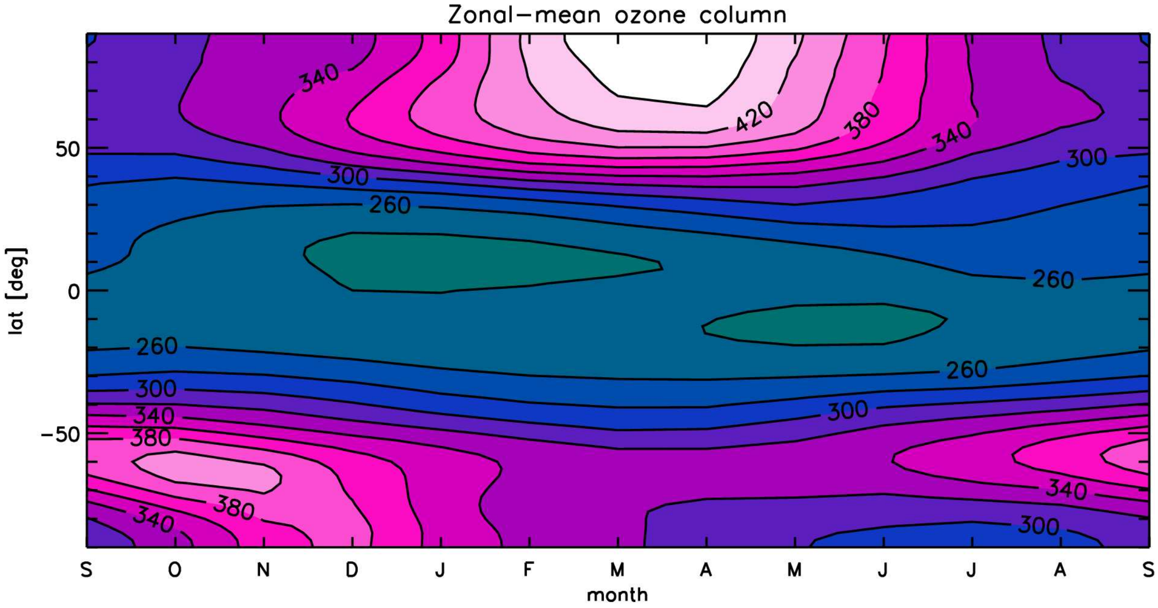


Figure 10: Mean annual zonal- and monthly mean ozone column (in Dobson Units), derived from the 10-year simulation (see text). The plot represents the average of the last 9 model years.

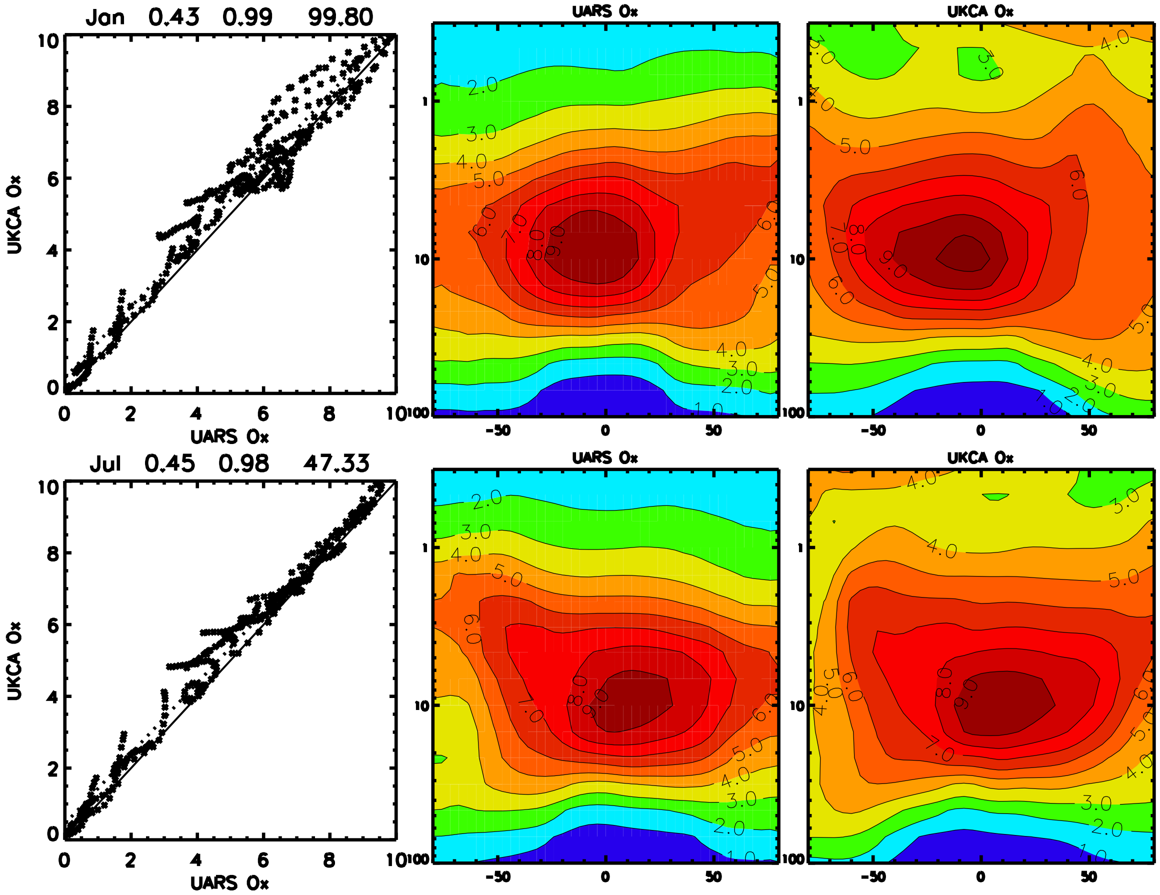


Figure 11: Zonal- and 9-year mean ozone mixing ratio (ppmv) for January (top) and July (bottom): (left) Scatter plots of UKCA versus UARS/HALOE climatology, The scatter plots only include points with $p > 2$ hPa and $|$ lat $| < 80^o$, (centre) UARS climatology, (right) UKCA 9-year mean.

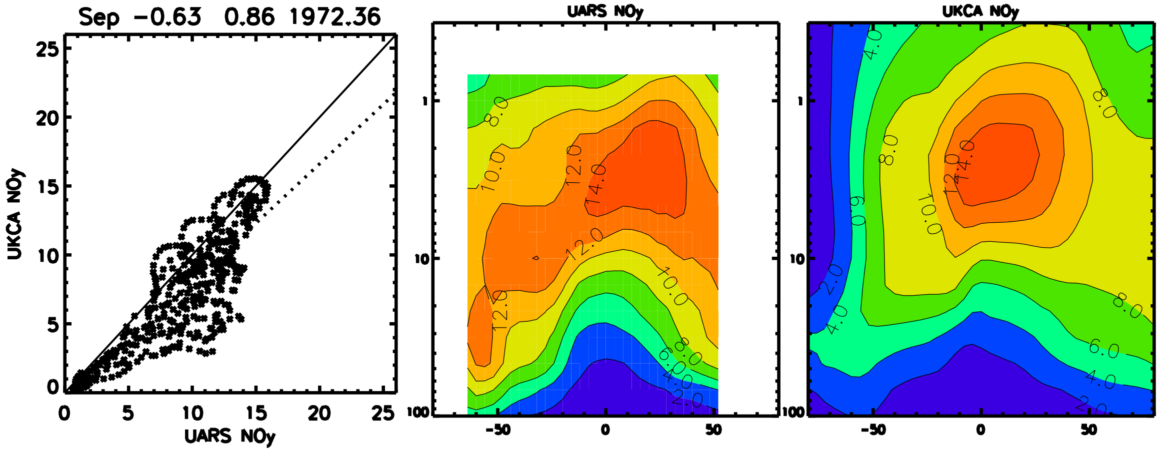


Figure 12: Zonal mean odd nitrogen (NO + NO_2 + $HONO_2$) (ppbv) in September, (centre) UARS climatology (right) UKCA.

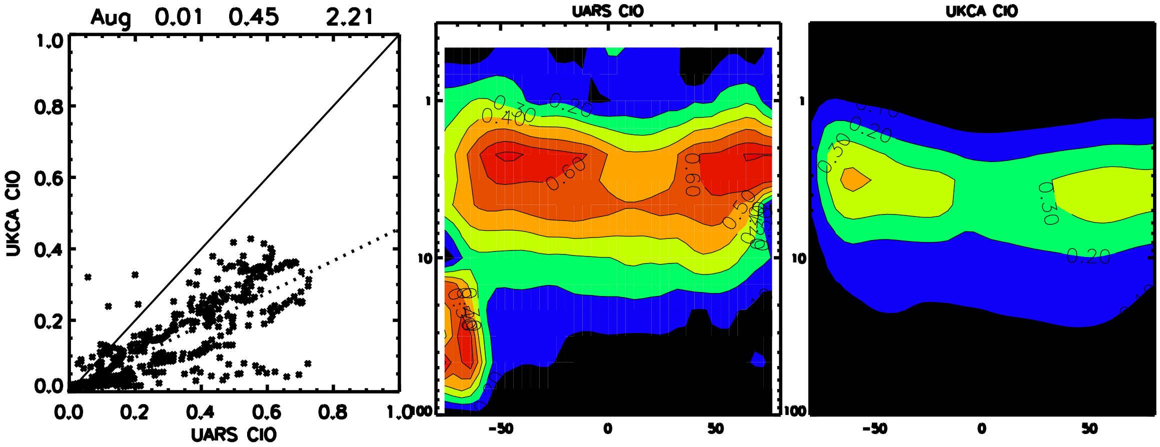


Figure 13: Zonal mean ClO (ppbv) in September, in (centre) UARS climatology (right) UKCA.

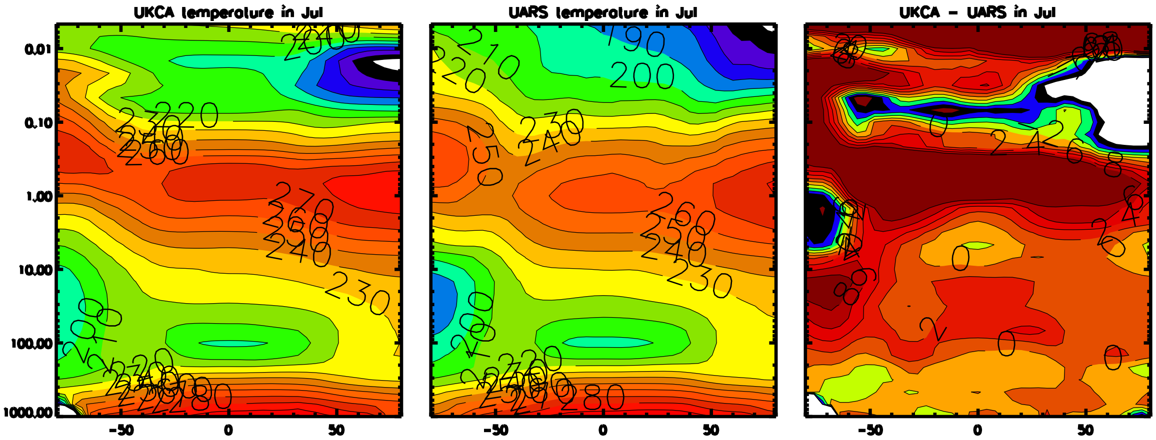


Figure 14: Zonal- and monthly mean temperature (K) in July: (left) UKCA, (centre) SPARC climatology, (right) Difference.

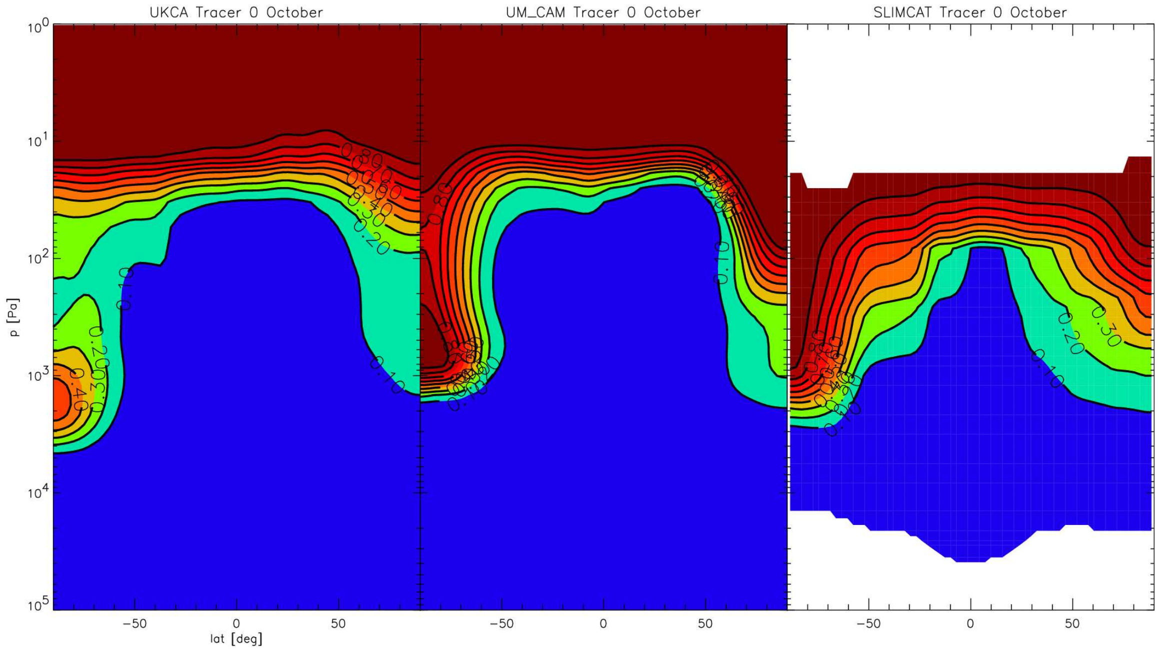


Figure 15: Zonal- and monthly mean mesospheric tracer mixing ratio in October (month 14 of the integration): (left) UKCA, (centre) UM 4.5 L60, (right) SLIMCAT.

Figure 14

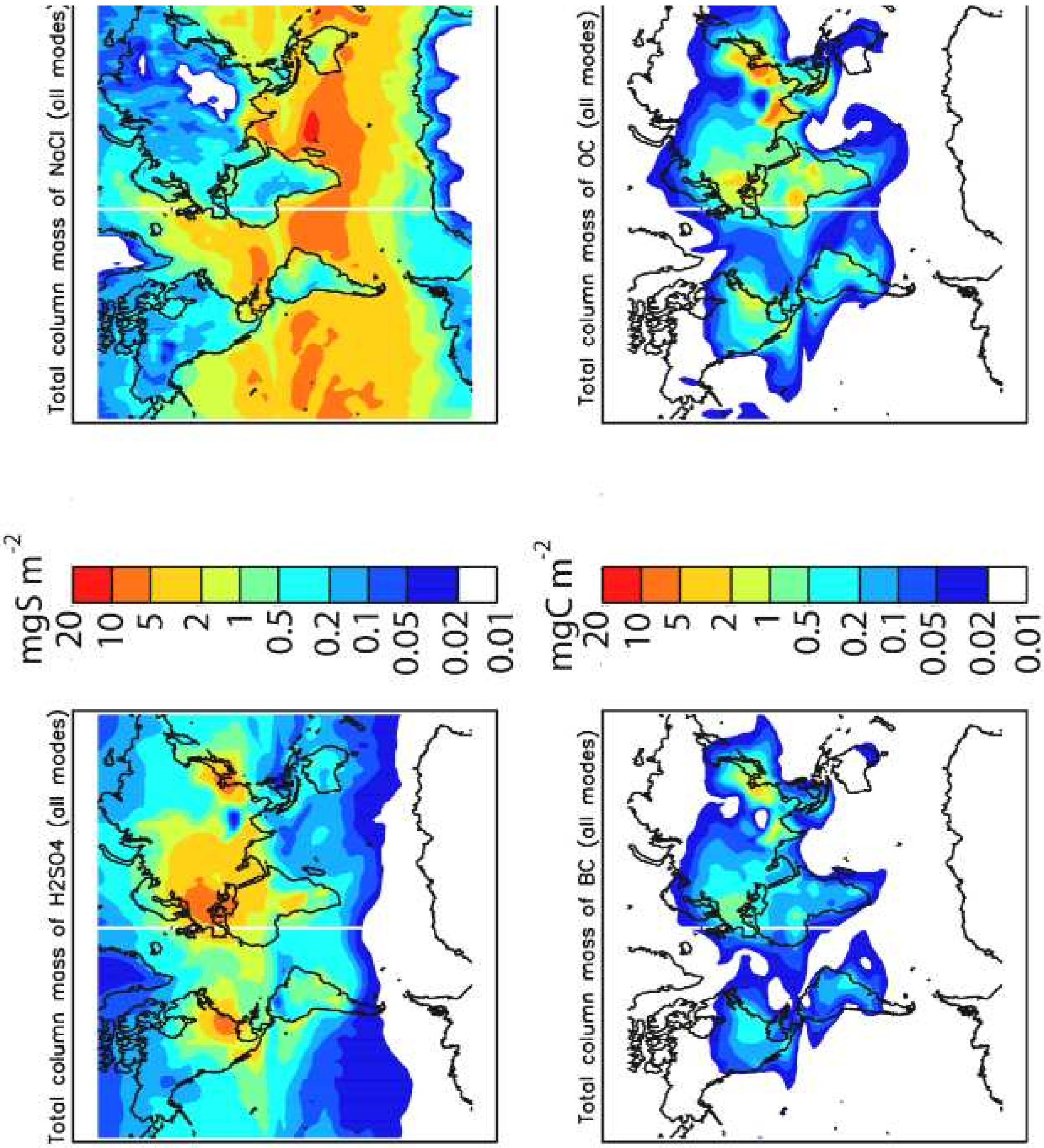


Figure 16: Total column masses of aerosol simulated in UKCA-MODE operating in the TOMCAT off-line model. Sulphate, sea-salt, black carbon and organic carbon are shown.

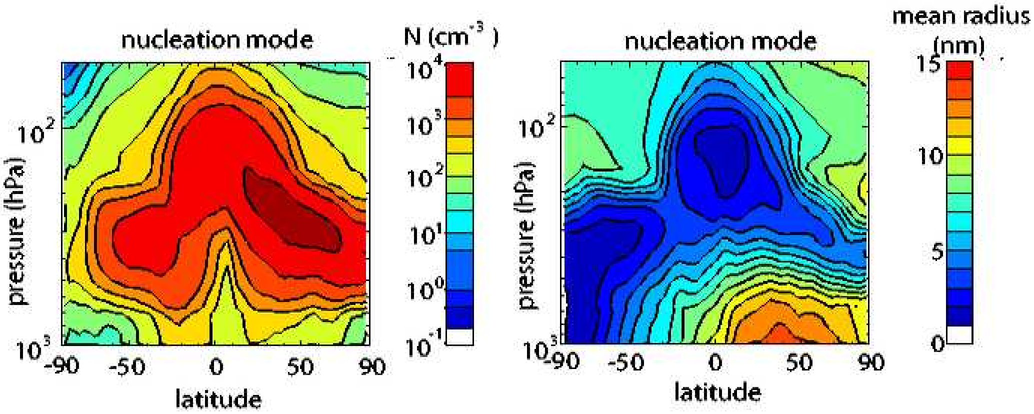
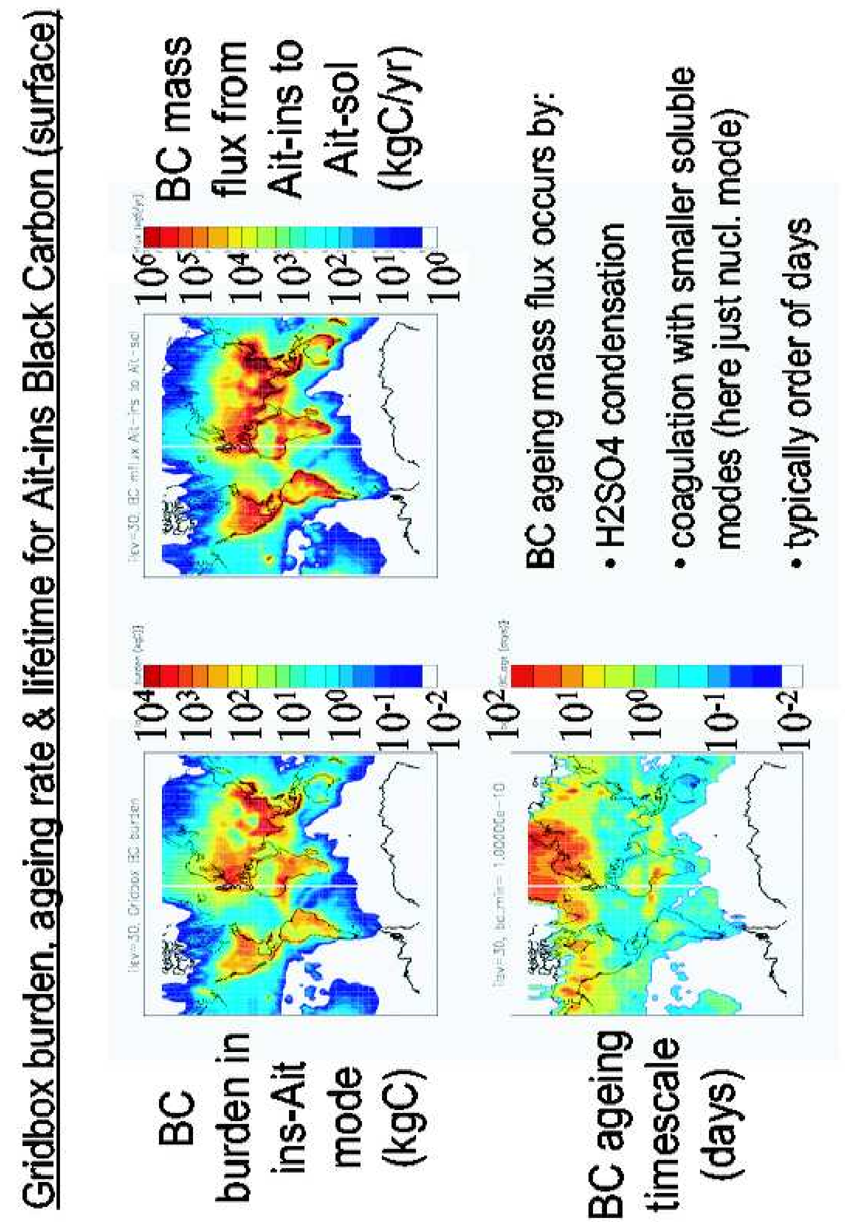


Figure 17: Zonal mean number density and mean radius for nucleation mode aerosol calculated by UKCA-MODE.



Gridbox burden, ageing rate & lifetime for Ait-ins Black Carbon (surface)

BC burden in ins-Ait mode (kgC)

BC ageing timescale (days)

BC mass flux from Ait-ins to Ait-sol (kgC/yr)

BC ageing mass flux occurs by:

- H2SO4 condensation
- coagulation with smaller soluble modes (here just nucl. mode)
- typically order of days

Figure 18: Black carbon burden, ageing rate and ageing lifetime calculated by UKCA-MODE.