Tropospheric Configuration of UKCA
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Transport

The United Kingdom Chemistry and Aerosol (UKCA) model has been coupled to the HadGEM family of Met Office Hadley Centre climate models (Johns et al., 2006; Martin et al., 2006; Collins et al., 2009), all of which are based on the U.K. Met Office's Unified Model (UM). As a result, UKCA uses components of the UM for the large-scale advection, convective transport, and boundary layer mixing of its chemical tracers. The large-scale transport is based on the new dynamical core implemented in the UM by Davies et al. (2005). The horizontal latitude-longitude grid in use is a staggered Arakawa C-grid (Arakawa and Lamb 1977) with typical climate model resolutions of N48 i.e. 2.5˚ latitude x 3.75˚ longitude or N96 i.e. 1.25˚ latitude x 1.875˚ longitude. A staggered Charney-Phillips grid is used in the vertical with either 38 levels (extending up to 40 km) or 60 levels (extending up to 83 km). Advection is semi-Lagrangian with conservative and monotone treatment of tracers (Davies et al., 2005). Convective transport is treated according to the mass-flux scheme of Gregory and Rowntree (1990) and is applicable to moist convection of all types (shallow, deep, and mid-level) in addition to dry convection. For boundary layer mixing, UKCA makes use of a new boundary layer turbulent mixing scheme (Lock et al., 2000) which includes a representation of non-local mixing in unstable layers and an explicit entrainment parameterization

Chemistry Schemes

The UM release at vn7.1 (+ branch) supports 3 tropospheric chemistry schemes (Table 1). The first chemistry scheme (Trop) includes NO_x-HO_x-CO-CH_4-O_3 chemistry with explicit treatment of ethane and propane and has previously been used in both the TOMCAT chemical transport model (Savage et al., 2004) and chemistry-climate integrations (Zeng and Pyle, 2003; Zeng and Pyle, 2005). This was included in an intercomparison of chemistry schemes and, unsurprisingly, was found to have a low photochemical ozone production potential due to its lack of higher non-methane hydrocarbons (Archibald, 2007). The second scheme (TropIsop) is an extension of the first scheme to include the 34 reactions of the Mainz Isoprene Mechanism (Poschl et al., 2000). This scheme was included in a recent chemical mechanism intercomparison by Emmerson and Evans (2008); it was found to show good agreement with the Master Chemical Mechanism (Jenkin et al., 2003; Saunders et al., 2003; Bloss et al., 2005) in simulating both O_3 and OH concentrations. The third scheme (Aerchem) is again an extension of the first scheme; in this case, it includes oxidation of SO_2 and DMS and provides input to the treatment of sulphate aerosol in UKCA-MODE, the aerosol component of UKCA. The choice of chemical scheme is controlled by UKCA logicals L_ukca_trop (Scheme 1), L_ukca_tropisop (Scheme 2), and L_ukca_aerchem (Scheme 3). In all 3 schemes, bimolecular and termolecular reaction rate co-efficients follow recommendations from IUPAC (2005), JPL (2003), and the Master Chemical Mechanism vn3.1 (http://www.chem.leeds.ac.uk/Atmospheric/MCM/mcmproj.html). Two additional schemes (RAQ and ExtTC) with more extensive treatment of non-methane hydrocarbons have been run within UKCA and are included in Table 1; these are not available with the UMvn7.1 release but could be added by means of an FCM branch.

	Trop	TropIsop = Trop+MIM	Aerchem = Trop + S	RAQ	ExtTC = TropIsop + VOCs
Tracers	26	40	27	40	60
Species	46	60	49	58	82
Ethane, Propane	Yes	Yes	Yes	Yes	Yes
Isoprene	No	Yes	Yes	Yes	Yes
Other non-CH_4 VOCs	No	No	No	Alkenes, Aromatics	Alkenes, Terpenes, Aromatics
Aerosol formation	No	No	Sulphate	No	SOA

Table1: Brief Summary of the various tropospheric chemistry schemes being run within UKCA. Some of these schemes are available as part of the UMvn7.1 release and others need to be added by means of an FCM branch.

Photolysis
In the UM code release at vn7.1, UKCA has two different treatments for photolysis. The first and simplest treatment, controlled by the UKCA logical L_ukca_phot2d, is where use is made of photolysis rates which have been calculated offline in the Cambridge 2D model (Law and Pyle, 1993) with the Hough (1988) scheme. These are read in by UKCA on the first time step of the model integration and interpolated in time and space at each model grid box. Although this treatment gives realistic diurnal and seasonal variations in photolysis rates, there is no variability associated with cloud cover and/or aerosol; the 2D rates were calculated with a climatological cloud cover and a prescribed aerosol loading. The second more sophisticated treatment is Fast-j (Wild et al., 2000) which provides a flexible and accurate scheme for the calculation of photolysis rates in the presence of both cloud and aerosol layers. In its implementation in UMvn7.1, the Fast-j scheme is only called when the UKCA logical L_ukca_fastj is set to true and the scheme itself is provided with optical depths from cloud liquid water, cloud frozen water, and sulphate aerosol from the HadGEM model. This can be altered to either extend the number of aerosol types considered from HadGEM or to use optical depths derived from UKCA-MODE aerosol distributions. The Fast-j code also includes flexibility for running on both scalar and vector platforms and in addition, load balancing code was introduced. Unfortunately, there are some memory problems associated with running Fast-j which have not yet been resolved.

Wet Deposition
The wet deposition scheme implemented in UKCA is the same scheme as was implemented and validated in the TOMCAT model by Giannakopoulos et al. (1999). Here, it makes use of the climate model's 3D convective and large-scale precipitation (both rainfall and snowfall), following a scheme originally developed by Walton et al.

(1988). The scheme uses the scavenging co-efficient values for HNO_3 proposed by Penner et al. (1991), which are scaled down according to the fraction of each species in the liquid phase determined by Henry's Law. Further evaluation of the scheme, particularly its UKCA implementation, can be found in O'Connor et al. (2009).

Dry Deposition
The tropospheric configuration of UKCA in UMvn7.1 supports two different dry deposition schemes. The first scheme is a very simple dry deposition scheme and is the default scheme. It assumes that the rate of dry deposition τ_d (s^{-1}) can be expressed as a function of the dry deposition velocity V_d ($m\ s^{-1}$) as follows:

$$\tau_d = V_d/H$$

where H represents the height of the lowest model layer (m). The scheme uses prescribed deposition velocities at 1 metre above the ground (Ganzeveld and Lelieveld, 1995; Giannakopoulos, 1998 and references therein; Sander and Crutzen 1996) which are dependent on surface type, season, and time of day. They are then extrapolated from 1 metre to the centre of the bottom grid box, according to Sorteberg and Hov (1996). The second dry deposition scheme in UKCA is the "big-leaf" multiple resistance model of Smith et al. (2000) and is similar in its implementation to that in the STOCHEM model (Sanderson et al., 2006). The multiple resistances considered represent a) transport of gas molecules from the boundary layer to the immediate vicinity of the absorbing surfaces (aerodynamic resistance), b) diffusion through the quasi-laminar boundary layer of air close to absorbing surfaces (quasi-laminar resistance) and c) removal of the gas from the atmosphere depending on the chemical and physical properties of the gas and the surface (surface resistance). The multiple resistances are calculated for each surface type within a grid box and are then combined to give a grid-box deposition velocity and a first order loss rate. This "big-leaf" dry deposition scheme is chosen when the UKCA logical L_ukca_intdd is set to true. An important difference between the two schemes is that the dry deposition loss rates are only applied in the bottom model level with the first scheme but applied in all model levels within the boundary layer with the second scheme. Therefore, it is recommended that L_ukca_intdd is set to true.

Emissions
Surface, aircraft, and lightning emissions are all treated in the tropospheric configuration of UKCA.

The majority of surface emissions are prescribed through UM single-level ancillary files as monthly mean emissions in kg (species) $m^{-2}\ s^{-1}$. These emissions can be time-varying over a number of years or time-varying over a single year which are used repeatedly through the model integration. Although the second chemistry scheme includes an isoprene degradation mechanism, there is no code yet in UMvn7.1 to provide interactive biogenic emissions. The only source of interactive surface emissions currently treated in UKCA is that of CH_4 from wetlands according to Gedney et al. (2004) although the complete hydrology code is not present at UMvn7.1. In terms of UKCA, the coding is complete and all that is required is the setting of the logical switch L_ukca_qch4inter to true. In this case, the user needs to ensure that the prescribed CH_4 emissions do not include a component from wetlands. In addition to surface emissions, UKCA considers emissions of NO_x from aircraft. These emissions

are also prescribed by means of a UM multi-level ancillary file which specifies monthly mean emissions in units of kg NO_2/gridbox/s. These are converted to kg (NO) m^{-2} s^{-1} before being added to the NO chemical tracer.

Lightning emissions of NO_x are interactive and are coupled to the climate model's convection scheme following the implementation from the TOMCAT model by Stockwell et al. (1999). The global distribution and frequency of lightning flashes are calculated using the parameterization of Price and Rind (1992) from the model's cloud top height. The amount of NO_x emitted is a linear function of the discharge energy (Chameides et al., 1977) which is 10 times lower from an intracloud flash than from a cloud-to-ground flash (Kowalczyk and Bauer 1982; Price et al., 1997). The ratio of IC to CG flashes follows Price and Rind (1993) and varies with latitude. This ratio and the flash frequencies are used to derive an emission rate which is scaled to give a global annual total of 5 Tg (N)/year.

Top Boundary Conditions
There are a number of options available at UMvn7.1 to treat boundary conditions at the top of the model. In particular, there are treatments for O_3, CH_4, and NO_y.

For O_3, one option is to overwrite it at pressures below 70 hPa using output from the Cambridge 2D model (Law and Pyle, 1993). However, the disadvantage with this method is that the output from the 2D model is only for a single year and may not be appropriate for a long transient model integration. An alternative option is to use the same ozone field (SPARC or Rosenlof climatology) that is used to drive the UM's radiation scheme (Edwards and Slingo, 1996) which evolves with time. In this case, O_3 is overwritten on model levels which are a fixed number of levels above the diagnosed tropopause. This second option is selected when L_use_umo3 is set to true in the ukca_stratf routine.

The UKCA CH_4 field also has a top boundary condition applied to it to take account of the lack of CH_4 oxidation in the stratosphere above the top of the domain of the L38 model in particular. This can be carried out in one of two ways. The original method is similar to the first method for O_3, in that CH_4 is simply overwritten above 70 hPa with output from the Cambridge 2D model. However, this approach appears to be too strong a sink for CH_4 in the present day and acts as a source of CH_4 in the pre-industrial period! The alternative approach is to call a subroutine ukca_ch4_stratloss (not included in the UMvn7.1 release), in which an explicit loss rate is applied to CH_4 in the top levels of the model. The loss rate used should give a stratospheric loss of approximately 40 Tg (CH_4)/year in present-day simulations, in line with Prather et al. (2001).

As is the case for O_3 and CH_4, there are 2 alternative treatments for NO_y at the top boundary. In the first approach, NO_y output from the 2D Cambridge model is used to overwrite all the NO_y species in UKCA while still retaining their original partitioning. The second approach is that used in the STOCHEM model, in which a fixed O_3:HNO_3 ratio from Murphy and Fahey (1994) is used to simply overwrite HNO_3. All other NO_y species are not overwritten. The default approach is the first one but can be switched to the second method by setting L_use_O3HNO3ratio to true.

Such top boundary conditions will not be required when whole-atmosphere chemistry modelling within UKCA becomes more established.

References

Arakawa, A. and Lamb, V. R., Computational design of the basic dynamical processes of the UCLA general circulation model, Methods Comput. Phys., 17, 173-265, 1977.

Archibald, A., Tropospheric chemistry mechanisms: Assessment of the chemistry mechanisms used in NAME and UKCA, Report, 2007.

Bloss, C., Wagner, V., Jenkin, M. E., Volkamer, R., Bloss, W. J., Lee, J. D., Heard, D. E., Wirtz, K., Martin-Reviejo, M., Rea, G., Wenger, J. C., and Pilling, M. J., Development of a detailed chemical mechanism (MCMv3.1) for the atmospheric oxidation of aromatic hydrocarbons, Atmos. Chem. Phys., 5, 641-664, 2005.

Chameides, W. L., Stedman, D. H., Dickerson, R. R., Rusch, D. W., and Cicerone, R. J., NO_x production in lightning, J. Atmos. Sci., 34, 143-149, 1977.

Collins, W. J., Bellouin, N., Doutriaux-Boucher, M., Gedney, N., Halloran, P., Hinton, T., Jones, C. D., Liddicoat, S., Martin, G., O'Connor, F., Rae, J., Senior, C., Totterdell, I., Woodward, S., Reichler, T., and Kim, J., Evaluation of the HadGEM2 model, *Hadley Centre Tech. Note 74*, 2009.

Davies, T., Cullen, M. J. P., Malcolm, A. J., Mawson, M. H., Staniforth, A., White, A. A., and Wood, N., A new dynamical core for the Met Office's global and regional modelling of the atmosphere, Q. J. R. Meteorol. Soc., 131, 1759-1782, 2005.

Edwards, J. M. and Slingo, A., Studies with a flexible new radiation code. I: Choosing a configuration for a large-scale model, Q. J. R. Meteorol. Soc., 122, 689-719, 1996.

Emmerson, K. M. and Evans, M. J., Comparison of tropospheric chemistry schemes for use within global models, Atmos. Chem. Phys. Discuss., 8, 19957-19987, 2008.

Ganzeveld, L. and Lelieveld, J., dry deposition parameterization in a chemistry general-circulation model and its influence on the distribution of reactive trace gases J. Geophys. Res., 100, D10, 20999-21012, 1995.

Gedney, N., Cox, P. M., and Huntingford C., Climate feedback from wetland methane emissions, Geophys. Res. Lett., 31, 20, L20503, doi:10.1029/2004GL020919, 2004.

Giannakopoulos, C., Three dimensional modelling of the concentration and deposition of tropospheric trace gases, Ph.D. thesis, University of Cambridge, U.K., 1998.

Giannakopoulos, C., Chipperfield, M. P., Law, K. S., and Pyle, J. A., Validation and intercomparison of wet and dry deposition schemes using ^{210}Pb in a global three-dimensional off-line chemistry model, J. Geophys. Res., 104, D19, 23761-23784, 1999.

Gregory, D. and Rowntree, P. R., A mass flux scheme with representation of cloud ensemble characteristics and stability-dependent closure, Mon. Wea. Rev., 118, 1483-1506, 1990.

Hough, A. M., The calculation of photolysis rates for use in global tropospheric modelling studies, AERE Report, 13259, At. Energy Res. Estab., Harwell, U.K., 1988.

IUPAC Subcommittee for Gas Kinetic Data Evaluation. Summary of evaluated kinetic data and photochemical data for atmospheric chemistry, March 2005 (plus data sheets). All at: http://www.iupac-kinetic.ch.cam.ac.uk/.

Jenkin, M. E., Saunders, S. M., Wagner, V., and Pilling, M. J., Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part B): tropospheric degradation of aromatic volatile organic compounds, Atmos. Chem. Phys., 3, 181-193, 2003.

JPL Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies. Evaluation Number 14, JPL Publication 02-25, February 2003. From: http://jpldataeval.jpl.nasa.gov/, 2003.

Johns, T. C., Durman, C. F., Banks, H. T., Roberts, M. J., McLaren, A. J., Ridley, J. K., Senior, C. A., Williams, K. D., Jones, A., Rickard, G. J., Cusack, S., Ingram, W. J., Crucifix, M., Sexton, D. M. H., Joshi, M. M., Dong, B.-W., Spencer, H., Hill, R. S. R., Gregory,J. M., Keen, A. B., Pardaens, A. K., Lowe, J. A., Bodas-Salcedo, A., Stark, S., and Searl, Y., The new Hadley Centre climate model HadGEM1: evaluation of coupled simulations, J. Climate, 19, 1302-1328, 2006.

Kowalczyk, M. and Bauer, E., Lightning as a source of NO in the troposphere, Rep. FAA-EE-82-4. U.S. Department of Transport, Washington, DC., USA, 1982.

Law, K. S. and Pyle, J. A., Modelling trace gas budgets in the troposphere. 1. ozone and odd nitrogen, J. Geophys. Res., 98, 18377-18400, 1993.

Lock, A. P., Brown, A. R., Bush, M. R., Martin, G. M., and Smith, R. N. B., A new boundary layer mixing scheme. Part I: Scheme description and single-column model tests, Mon. Wea. Rev., 128, 3187-3199,2000.

Martin, G. M., Ringer, M. A., Pope, V. D., Jones, A., Dearden, C., and Hinton, T. J., The physical properties of the atmosphere in the new Hadley Centre Global Environmental Model (HadGEM1). Part I: model description and global climatology, J. Climate, 19, 1274-1301, 2006.

Master Chemical Mechanism vn3.1, At: http://www.chem.leeds.ac.uk/Atmospheric/MCM/mcmproj.html.

Murphy, D. and Fahey, D., An estimate of the flux of stratospheric reactive nitrogen and ozone into the troposphere, J. Geophys. Res., 99, D3, 5325-5332, 1994.

O'Connor, F. M., et al. Evaluation of the new UKCA climate-composition model. Part 2: The troposphere, *Geosci. Model Develop.*, In preparation, 2009.

Penner, J. E., Atherton, C. S., Dignon, J., Ghan, S. J., and Walton, J. J., Tropospheric nitrogen: A three-dimensional study of sources, distributions and deposition, J. Geophys. Res., 96, 959-990, 1991.

Poschl, U., von Kuhlmann, R., Poisson, N., and Crutzen, P. J., Development and intercomparison of condensed isoprene oxidation mechanisms for global atmospheric modelling, J. Atmos. Chem., 37, 1, 29-52, 2000.

Prather, M. J., et al., Atmospheric chemistry and greenhouse gases, in Climate Change 2001: The Scientific Basis. Contribution of Working Group I to the Third Assessment Report of the Intergovernmental Panel on Climate Change (IPCC), edited by J. T. Houghton et al., 881 pp., Cambridge Univ. Press, New York, 2001.

Price, C. and Rind, D., A simple lightning parameterization for calculating global lightning distributions, Geophys. Res. Lett., 97, 9919-993, 1992.

Price, C. and Rind, D., What determines the cloud-to-ground lightning fraction in thunderstorms?, Geophys. Res. Lett., 20, 463-466, 1993.

Price, C., Prather, M., and Penner, J. E., NO_x from lightning. Part I: global distribution based on lightning physics, J. Geophys. Res., 102, 5929-5941, 1997.

Sander, R. and Crutzen, P., Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea, J. Geophys. Res., 101, D4, 9121-9138, 1996.

Sanderson, M. G., Collins, W. J., Johnson, C. E., and Derwent, R. G., Present and future acid deposition to ecosystems: The effect of climate change, Atmos. Environ., 40, 1275-1283, 2006.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J., Protocol for the development of the Master Chemical Mechanism, MCM v3 (Part A): tropospheric degradation of non-aromatic volatile organic compounds, Atmos. Chem. Phys., 3, 161-180, 2003.

Savage, N. H. , Law, K. S., Pyle, J. A., Richter, A., Nuss, H., and Burrows, J. P., Using GOME NO_2 satellite data to examine regional differences in TOMCAT model performance, Atmos. Chem. Phys., 4, 1895-1912, 2004.

Smith, R. I., Fowler, D., Sutton, M. A., Flechard, C., and Coyle, M., Regional estimation of pollutant gas dry deposition in the UK: model description, sensitivity analyses and outputs, Atmos. Environ., 34, 3757-3777, 2000.

Sorteberg, A. and Hov, O., Two parametrizations of the dry deposition exchange for SO_2 and NH_3 in a numerical model., Atmos. Environ., 30, 10/11, 1823-1840, 1996.

Stockwell, D. Z., Giannakopoulos, C., Plantevin, P.-H., Carver, G. D., Chipperfield, M. P., Law, K. S., Pyle, J. A., Shallcross, D. E., and Wang, K.-Y., Modelling NO_x from lightning and its impact on global chemical fields, Atmos. Environ., 33, 4477-4493, 1999.

Walton, J. J., McCracken, M. C., and Ghan, S. J., A global scale Lagrangian trace species model of transport, transformation, and removal processes, J. Geophys. Res., 93, 8339-8354, 1988.

Wild, O., Zhu, X., and Prather, M. J., Fast-J: Accurate simulation of in- and below-cloud photolysis in tropospheric chemical models, J. Atmos. Chem., 37, 245-282, 2000.

Zeng G. and Pyle, J. A., Changes in tropospheric ozone between 2000 and 2100 modeled in a chemistry-climate model, Geophys. Res. Lett., 30, 7, 1392, doi:10.1029/2002GL016708, 2003.

Zeng G. and Pyle, J. A., Influence of El Nino Southern Oscillation on stratosphere/troposphere exchange and the global tropospheric ozone budget, Geophys. Res. Lett., 32, 1, L01814, doi:10.1029/2004GL021353, 2005.