Unified Model

United Kingdom Chemistry and Aerosol (UKCA) Technical Description

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Contents

1 Introduction

UKCA (United Kingdom Chemistry and Aerosols) is a framework for atmospheric chemistry and aerosols operating in the MetUM environment using standard MetUM prognostics and diagnostics. It is designed to operate a variety of chemistry and aerosol schemes, together with the associated interactions between UKCA schemes and other components such as the radiation and carbon cycle schemes. UKCA was developed as a community model, in a collaboration between NCAS and The Met Office, with components provided by contributors from The University of Cambridge, University of Leeds, University of Oxford and The Met Office.

A variety of chemistry and aerosol configurations of UKCA are available. The purpose of this document is to provide a brief introduction to the features available, and to provide a short technical description.

Please contact the developers if you encounter any difficulties as it is not possible to test all of the many different configurations of UKCA which are possible. The UKCA web site will contain any updates which are advisable.

2 Prognostic and diagnostic variables

UKCA occupies four sections of the MetUM: section 34 (tracers); section 38 (aerosol diagnostics); section 50 (chemistry diagnostics); and section 37 (UKCA lateral boundary conditions). Each section currently contains a maximum of 999 items. These are allocated as shown in table 1. All of the prognostic advected tracers in use for both aerosols and chemistry are contained in section 34, with a maximum number of 150 tracers allowed. Some short-lived species in the chemical schemes are not transported, but are retained in the atmosphere dump file as non-advected prognostics. Other quantities (like the tropospheric heterogeneous rates) are required for the next timestep, so are also retained in the dump.

While the UM sets up the active tracers correctly for the RAQ scheme, some of the names of the tracers in the STASHmaster are incorrect unless a userSTASHMASTER file is used.

Tracer matching for the GLOMAP_mode aerosol scheme is done in routine UKCA_AERO_TRACER_INIT contained in module UKCA_MODE_SETUP. This creates indices to the UKCA tracer array using the selected modes and components. Each tracer is given a title in the STASHmaster file, but these are not available to the code, and are therefore mirrored (in an abbreviated form) in the nm_spec array held in routine ukca_set_nmspec. UKCA_AERO_TRACER_INIT uses the contents of nm_spec to identify the tracers to set the index arrays nmr_index and mmr_index for number and components. It is vital that any changes to the STASHmaster file are also made to the the nm_spec array.

2.1 UKCA specific option codes

As of UM9.0 the active UKCA tracers are calculated at run time by the model and not specified by a list of 1s and 0s. This is done by use of option codes in the STASHmaster file.

The option code is a 30-digit decimal code which defines under what conditions an item is available to STASH. The digits are labelled from left to right n30,n29,. . . ,n1.

If the option code is all zeros, the item is always available (to preserve compatibility with other sections). If the option code is non zero and UKCA is not on then the item is never available.

Table 1: Summary of section 34 and 38 prognostics and diagnostics.

Section/ Items	No. of items	Quantity	STASHmaster Codes
34 1-150	150	Advected Tracers	Halo = 1 (single point) Space= 2 (in dump) Option=nnn
34 151-179	29	Non-advected tracers and diags. needed in dump	Halo = 3 (none) Space = 2 (in dump) Option = 000
34 180-230	51	Emissions Not yet in use	Halo = 3 (none) Space= 2 (in dump)
34 231-512	282	Not yet in use	Halo = 3 (none) Space= 0 (not in dump)
38 151-200	50	Aerosol Emissions Not yet in use	Halo = 3 (none) Space= 2 (in dump)
38 200-512	313	GLOMAP Diagnostics	Halo = 3 (none) Space= 0 (not in dump)
50 1-512	512	Chem. Diagnostics	Halo = 3 (none) Space= 0 (not in dump)

If UKCA is on then the code first tests the value of n30 to establish whether the item depends on the chemistry scheme or the aerosol configuration.

If n30=0, the availability of this item depends on the chemistry scheme in use. The code then tests the value of a specific option code depending on the chemistry. If the checked option code is zero, then the item is not available. If it is 1 then is available. If it is 2 then it is only available when using the extension to chemistry for aerosol modelling. This is the list of which option codes are tested for which chemistry schemes.

- n1 = age of air.
- n2 = BE Tropospheric
- n3 = BE RAQ
- n4 = NR TropIsop
- n5 = NR StratTrop
- n6 = NR Strat

If n30 = 1 the availability of this item depends on the set up of the GLOMAP-mode aerosol scheme in use. If GLOMAP-mode is off the item is not available. The code then tests the value of a specific option code depending on the value of i_mode_setup. If the checked option code is zero, then the item is not available. If it is 1 then it is available.

- n1 = i_mode_setup = 1
- n2 = i_mode_setup = 2

To add or remove a tracer from a chemistry or aerosol scheme, it is just necessary to change the value of the option code for that tracer in the STASHmaster file. If a complete new scheme is being added, the developer needs to choose a new option code for that scheme and then add the logic for it in the subroutine tstmsk_ukca.F90.

3 Interface with UM Atmosphere

UKCA is a component of the MetUM atmosphere, with tracer advection and convective tracer transport being handled by the MetUM. UKCA is called from the routine U_MODEL after the atmosphere step. The model fields required to run UKCA are taken from standard prognostics and diagnostics and are made available at each timestep. Each diagnostic is current at the timestep, and is placed in the D1 array secondary store. Diagnostics are held with an associated tag (98). UKCA reads the required items from secondary store, reshapes each array and places it in an allocated array.

3.1 Interface code

The items required by UKCA are specified in the UKCAD1CODES array which is a structure with the following components: SECTION, ITEM, N_LEVELS, ADDRESS, LENGTH, HALO_TYPE, GRID_TYPE, FIELD_TYPE, LEN_DIM1, LEN_DIM2, LEN_DIM3 (integers), together with logicals PROGNOSTIC and REQUIRED. The UKCAD1CODES array is held in the module UKCA_D1_DEFS, together with other initialised integers. The prognostic and diagnostic items used by UKCA are listed in tables 29 and 30 in Appendix B.

The items referenced in the UKCAD1CODES array are composed of the tracers, non-advected species, emissions, prognostics, and diagnostics. The section and item numbers are set in the routine UKCA_SETD1DEFS, together with the array lengths expected (not including any halo). The UKCA_SETD1DEFS routine is called only on the first timestep. For items used to drive UKCA, the logical variable REQUIRED is set to true. The diagnostics which are output from UKCA are also referenced in the UKCAD1CODES array, but with REQUIRED set to false. For diagnostic output, item numbers are set to missing data unless STASH requests have been set.

The UKCA_MAIN1 subroutine searches through the D1 array entries for prognostics or diagnostics which match the entries in the UKCAD1CODES array. When these are found, the other items in this array (N_LEVELS, ADDRESS, LENGTH, etc) are set from the D1_ADDR array. After the UKCAD1CODES array has been filled the routine GETD1FLDS is called for each item.

The GETD1FLDS subroutine has an entry for each item, and calls the routine UKCA_SET_ARRAY_BOUNDS to give the dimensions of each array, taking into account the halo sizes which have been read in from the D1_ADDR array. The required array can then be allocated using these sizes. A call to the generic rountine UKCA_EXTRACT_D1_DATA allows calls to the appropriate subroutine depending on the dimensions and type of data. The extraction routines copy the required data from the D1 array and reshape it to the required dimensions. Arrays which have halos are allocated with dimensions (1-halox:row_length+halox,1-haloy:rows+haloy), where halox and haloy are the haloes in the x and y directions.

At the end of the UKCA code, the routine PUTD1FLDS writes the tracer array back to D1. The chem_diags array is also written to D1, as this may contain the "non-advected" tracers from the chemistry.

If water vapour feedback from the chemistry is turned on, the water vapour array is also written back to D1.

Diagnostics from UKCA are copied into stashwork arrays via calls to the COPYDIAG_3D routine, and subsequently STASH is called for sections 34, 38 and 50.

3.2 Error handling and checking

If any required items were not found in the D1 array the model will stop through a call to EREPORT with the message:
"Item address not found in D1 array", with an error code equal to the STASH number of the item. If this occurs, check that the item is included in the STASH requests.

If the size of the allocated array does not correspond with the length of the item in D1, the extract routine will stop the model through a call to EREPORT with the message:
"Array sizes in local variable and D1 do not agree", with an error code equal to the position of the item in the UKCAD1CODES array. In this case check that the dimensions of the variable have been declared correctly in the routine UKCA_SETD1DEFS.

If the routine GETD1FLDS does not identify the STASH number, the model will stop through a call to EREPORT with a message: *"N not found in diagnostic(?) case statement"*, where ? is the STASH section, and the error code is the position in the UKCAD1CODES array. In this case, code for the field will need to be added to GETD1FLDS.

When the print status of the UM is set to be greater than "operational", the subroutine UKCA_SETD1DEFS will write variables (i.e. stash numbers, array length, etc.) from the UKCAD1CODES array to unit 6. On the first timestep and when print status is greater or equal to "operational", the routine UKCA_MAIN1 will write out minimum and maximum values from all the prognostic and diagnostic fields used by UKCA to unit 6.

4 Chemical schemes

A number of chemical schemes are available for UKCA, and these are summarised in table 2. Those based around the backward-Euler solver are still available for use, but are only briefly described here. Other schemes use the Newton-Raphson solver within the ASAD framework, and each of these schemes has an appropriate aerosol chemistry which is switched on if the GLOMAP-mode aerosol scheme is activated. Each scheme is fully described in a Fortran module. Note that the "extended" tropospheric chemistry (extTC) is not included in the trunk at present. At UMvn8.4, the reaction rate co-efficients for the Strat-trop (CheST) chemistry scheme were updated using more recent recommendations and hence, are no longer consistent with those of the other schemes.

The main namelist variable which controls the choice of chemistry scheme is the integer i_ukca_chem. i_ukca_chem=0 indicates that there is no chemistry at all, a value of 1 is used for age of air only simulations. The other values are indicated in table 2 in the column "integer code".

In addition three extra logicals can be used with certain chemistry schemes. These turn on additional reactions and/or species. To support aerosols the namelist contains a logical l_ukca_chem_aero. For N-R schemes this sets L_ukca_achem to true and for the B-E standard tropospheric scheme this sets the L_ukca_aerchem to true. Heterogeneous/PSC chemistry is turned on (available for N-R Std

Stratospheric, and N-R Strat-trop) by the L_UKCA_HET_PSC logical and tropospheric heterogeneous chemistry (available for N-R TropIsop, and N-R Strat-trop) using the logical L_UKCA_TROPHET.

The swich L_UKCA_ADVH2O set if water vapour is treated as an advected tracer in N-R schemes is automatically set to true for strat-trop and strat schemes and is not an input to the model.

Table 2: Summary of chemical schemes. The choice of scheme is set using the namelist integer value i_ukca_chem. Solver method is either backward-Euler (B-E) or Newton-Raphson (N-R) depending on the choice of scheme. For the N-R solver, an aerosol chemistry appropriate for either (or both) tropospheric or stratospheric conditions can be selected by the l_ukca_chem_aero logical. This logical can also be used to choose a version of the Standard tropospheric scheme with aerosol chemistry.

Name	No. Tracers	No. Species	No. Reactions	Solver	Logical Name	Integer code
Std Tropospheric (StdTrop)	26	46	129	B-E	L_ukca_trop	11
StdTrop + aerosol chemistry	33	53	164	B-E	L_ukca_aerchem	11
Regional Air Quality	40	58	215	B-E	L_ukca_raq	13
Trop-isoprene (TropIsop)	49	56	167	N-R	L_ukca_tropisop	50
TropIsop + aerosol chemistry	60	67	182	N-R	L_ukca_tropisop + L_ukca_achem	50
Std Stratospheric (Strat)	37	41	169*	N-R	L_ukca_strat	51
Strat + aerosol chemistry	45	49	189*	N-R	L_ukca_strat + L_ukca_achem	51
Strat-trop (CheST)	71	75	283*	N-R	L_ukca_strattrop	52
Strat-trop + aerosol chemistry	82	86	306*	N-R	L_ukca_strattrop + L_ukca_achem	52

The chemical schemes can be selected with rose edit and use the logical variables described in tables 2 and 32. *Please note that for these schemes, the number of reactions in the table is based on the assumption that L_ukca_trophet is false and L_ukca_het_psc is true.

4.1 Standard Tropospheric Chemistry

This chemical scheme is designed for climate studies and contains essential inorganic chemistry together with the chemistry for the degradation of methane, ethane, and propane. The chemistry is based on that of Law and Pyle (1993). Twenty six tracers are used, and there are thirteen non-advected species in addition. These are held in the dump and used to intialise the solver, in order to improve the solver accuracy. Tables 3 and 4 show the species included in this scheme, and also indicates the species with emissions, and those involved in dry and wet deposition processes. The solver for this scheme is an explicit iterative Backward-Euler, see section 6.2. The routine UKCA_DERIV holds the solver for this scheme, and UKCA_CHEMCO holds the relevant rate coefficients.

Table 3: Advected tracers treated by the standard tropospheric chemistry scheme.

Item	Tracer name	STASH	Name	Dry	Wet	Emitted
1	O3	34001	O_3	Yes		
2	NO	34002	NO	Yes		Yes
3	NO3	34003	NO_3	Yes	Yes	
4	NO2	34004	NO_2	Yes		Yes
5	N2O5	34005	N_2O_5	Yes	Yes	
6	HO2NO2	34006	HO_2NO_2	Yes	Yes	
7	HONO2	34007	$HONO_2$	Yes	Yes	
8	H2O2	34008	H_2O_2	Yes	Yes	
9	CH4	34009	CH_4	Yes		Yes
10	CO	34010	CO	Yes		Yes
11	HCHO	34011	HCHO	Yes	Yes	Yes
12	MeOOH	34012	CH_3OOH	Yes	Yes	
13	HONO	34013	HONO	Yes	Yes	
14	C2H6	34014	C_2H_6			Yes
15	EtOOH	34015	C_2H_5OOH	Yes	Yes	
16	MeCHO	34016	CH_3CHO	Yes		Yes
17	PAN	34017	$CH_3O_3NO_2$	Yes		
18	C3H8	34018	C_3H_8	Yes		Yes
19	n-PrOOH	34019	n-C_2H_7OOH	Yes	Yes	
20	i-PrOOH	34020	i-C_2H_7OOH	Yes	Yes	
21	EtCHO	34021	CH_3CHO	Yes		
22	Me2CO	34022	CH_3COCH_3			Yes
23	MeCOCH2OOH	34023	CH_3COCH_2OOH	Yes	Yes	
24	PPAN	34024	$C_2H_5CO_3NO_2$	Yes		
25	MeONO2	34025	CH_3ONO_2			
26	O3S	34026	O_3 (Stratospheric)	Yes		

4.2 Tropospheric chemistry with parameterised Isoprene scheme

This scheme uses the species shown in tables 3 and 4, with only $O(^1D)$ and $O(^3P)$ being treated in steady state, the rest being advected tracers. Stratospheric O_3, OH, and HO_2 are not included in this scheme. An extra 15 tracers (table 5) are used for the MIM condensed isoprene scheme and for CH_3OH. The isoprene tracers and chemistry are described in Pöschl et al. (2000).

4.3 Chemistry for Regional Air Quality (RAQ)

This tropospheric chemistry scheme has a larger chemical mechanism that that of the standard tropospheric chemistry scheme and was created for use in regional air quality modelling applications of the MetUM. It involves 40 tracers (16 of them emitted), 23 photolysis reactions and $\sim$ 115 gas-phase reactions. Removal by wet and dry deposition are considered for 19 and 16 species, respectively. Unlike the standard tropospheric chemistry, this scheme includes the oxidation of both C2-C3 alkenes (ethene and propene) and aromatic compounds such as toluene and o-xylene as well as the formation of organic

Table 4: Non-advected tracers treated by the standard tropospheric chemistry scheme.

Item	Tracer name	STASH	Name	Dry	Wet	Emitted
1	O3P	34151	$O(^3P)$			
2	O1D	34152	$O(^1D)$			
3	OH	34153	OH			
4	HO2	34154	HO_2		Yes	
5	MeOO	34155	CH_3O_2		Yes	
6	EtOO	34156	$C_2H_5O_2$			
7	MeCO3	34157	CH_3COO_2			
8	n-PrOO	34158	n-$C_2H_7O_2$			
9	i-PrOO	34159	i-$C_2H_7O_2$			
10	EtCO3	34160	$C_2H_5COO_2$			
11	MeCOC2OO	34161	$CH_3COC_2O_2$			
12	OHS	34162	OH (Stratospheric)			
13	HO2S	34163	HO_2 (Stratospheric)		Yes	

nitrate. However it does not include HONO, which plays a role in urban-scale photochemistry. It is adapted from the mechanism presented in Collins et al. (1997) with the additional reactions described in Collins et al. (1999). Note however that sulphur chemistry is not included in the RAQ mechanism. As with the standard tropospheric chemistry there are non-advected species which are held in the dump and used to intialise the solver, in order to improve the solver accuracy. Some of these are the same as in the standard tropospheric chemistry but there are 18 fields in total. Tables 6 and 7 show the species included in this scheme, and also indicates the species with emissions, and those involved in dry and wet deposition processes. Sulphur and ammonia chemistry is not included in this scheme yet.

The solver for this scheme is an explicit iterative Backward-Euler, see section 6.2. Routine UKCA_DERIV_RAQ holds the solver for this scheme, and UKCA_CHEMCO_RAQ holds the relevant rate coefficients.

Table 5: Advected tracers treated by the parameterised isoprene scheme. See Pöschl et al. (2000) for descriptions of lumped species.

Item	Tracer name	STASH	Name	Dry	Wet	Emitted
1	C5H8	34027	C_5H_8			yes
2	ISOOH	34028		yes	yes	
3	ISON	34029		yes	yes	
4	MACR	34030		yes		
5	MACROOH	34031		yes	yes	
6	MPAN	34032		yes		
7	HACET	34033		yes	yes	
8	MGLY	34034		yes	yes	
9	NALD	34035		yes		
10	HCOOH	34036	$HCOOH$	yes	yes	
11	MeCO3H	34037	CH_3CO_3H	yes	yes	
12	MeCO2H	34038	CH_3COOH	yes	yes	
13	ISO2	34040	peroxy radicals			
14	MACRO2	34060	peroxy radicals			
15	MeOH	34090	CH_3OH			Yes

4.4 Stratospheric Chemistry

The stratospheric chemistry uses 37 tracers for the chemistry, with one tracer to represent the age of air, and another to represent advected passive ozone. Table 8 shows the tracer species, and indicates the species which are deposited and those emitted or subject to a lower boundary condition. In addition to the tracers, $O(^1D)$ is a steady state species treated as a diagnostic. The scheme is described by Morgenstern et al. (2009), with the minor changes of H_2 being treated as a tracer rather than as a constant field in the chemistry, and the heterogeneous reactions forming Cl rather than Cl_2O_2 or OClO.

Due to the problems with tracer conservation, all N, Br, and Cl containing species are lumped into tracers for advection purposes (using tracers labelled as Lumped N, Lumped Br, and Lumped Cl tracers in STASH items 98–100, respectively). The routine `UKCA_TRANSFORM_HALOGEN` is called to lump the species before advection (at the end of `UKCA_MAIN1`) and again before the chemistry to unlump them (at the beginning of `UKCA_MAIN1`). Due to this umlumping step, it is important to initialise the lumped species correctly (i.e., as lumped, rather than unlumped) to prevent initialisation problems. None of the lumped tracers have any chemical meaning, and should not be thought of in those terms. Diagnostic values of NO_2, BrO, and HCl are provided in section 34, items 153-155.

4.5 Chemistry for stratosphere and troposphere (CheST)

This chemistry is based on the stratospheric chemistry described above (section 4.4), together with the tropospheric chemistry with isoprene (section 4.2). The scheme was developed by adding to the stratospheric chemistry scheme. Relative to the stratospheric chemistry, extra emissions are provided for: C_2H_6 (ethane), C_3H_8 (propane) and C_5H_8 (isoprene).

The CheST scheme uses 69 chemical tracers, as well as including one tracer to represent the age of air, and one tracer to represent passive ozone. $O(^1D)$ is treated as a steady state species (as in the stratospheric chemistry). Table 9 shows the species list and whether the species are deposited, emitted or may require a lower boundary condition.

Table 9: Advected tracers and diagnostic species treated by the CheST chemistry scheme. The diagnostic species are $O(^1D)$, NO_2, BrO, and HCl.

	STASH name	STASH	UKCA Species	Dry	Wet	Emitted/Lower BC
1	O3	34001	$\mathrm{O_3}$	Yes		
2	NO	34002	NO			Emitted
3	NO3	34003	$\mathrm{NO_3}$	Yes	Yes	
4	N2O5	34005	$\mathrm{N_2O_5}$	Yes	Yes	
5	HO2NO2	34006	$\mathrm{HO_2NO_2}$	Yes	Yes	
6	HONO2	34007	$\mathrm{HONO_2}$	Yes	Yes	
7	H2O2	34008	$\mathrm{H_2O_2}$	Yes	Yes	
8	CH4	34009	$\mathrm{CH_4}$			Lower BC
9	CO	34010	CO	Yes		Emitted
10	HCHO	34011	HCHO	Yes	Yes	Emitted
11	MeOOH	34012	$\mathrm{CH_3OOH}$	Yes	Yes	
12	HONO	34013	HONO	Yes	Yes	
13	C2H6	34014	$\mathrm{C_2H_6}$			Emitted
14	EtOOH	34015	$\mathrm{C_2H_5OOH}$	Yes	Yes	
15	MeCHO	34016	$\mathrm{CH_3CHO}$	Yes		Emitted
16	PAN	34017	$\mathrm{CH_3O_3NO_2}$	Yes		
17	C3H8	34018	$\mathrm{C_3H_8}$	Yes		Emitted
18	n-PrOOH	34019	$\mathrm{n\text{-}C_2H_7OOH}$	Yes	Yes	
19	i-PrOOH	34020	$\mathrm{i\text{-}C_2H_7OOH}$	Yes	Yes	
20	EtCHO	34021	$\mathrm{CH_3CHO}$	Yes		
21	Me2CO	34022	$\mathrm{CH_3COCH_3}$			Emitted
22	MeCOCH2OOH	34023	$\mathrm{CH_3COCH_2OOH}$	Yes	Yes	
23	PPAN	34024	$\mathrm{C_2H_5CO_3NO_2}$	Yes		
24	MeONO2	34025	$\mathrm{CH_3ONO_2}$			
25	C5H8	34027	C_5H_8			Emitted
26	ISOOH	34028		Yes	Yes	
27	ISON	34029		Yes	Yes	
28	MACR	34030		Yes		
29	MACROOH	34031		Yes	Yes	
30	MPAN	34032		Yes		
31	HACET	34033		Yes	Yes	
32	MGLY	34034		Yes	Yes	
33	NALD	34035		Yes		
34	HCOOH	34036	$HCOOH$	Yes	Yes	
35	MeCO3H	34037	CH_3CO_3H	Yes	Yes	

Table 9: Advected tracers treated by CheST (continued)

	STASH name	STASH	UKCA Species	Dry	Wet	Emitted/Lower BC
36	MeCO2H	34038	CH_3COOH	Yes	Yes	
37	Specific Humidity	34039	H2O			
38	ISO2	34040	peroxy radicals			
39	Cl	34041	Cl			
40	ClO	34042	ClO			
41	Cl2O2	34043	$\mathrm{Cl_2O_2}$			
42	OClO	34044	OClO			
43	Br	34045	Br			
44	BrCl	34047	BrCl			
45	BrONO2	34048	$\mathrm{BrONO_2}$		Yes	
46	N2O	34049	$\mathrm{N_2O}$			Lower BC
47	HOCl	34051	HOCl		Yes	
48	HBr	34052	HBr		Yes	
49	HOBr	34053	HOBr		Yes	
50	ClONO2	34054	$\mathrm{ClONO_2}$		Yes	
51	CFCl3	34055	$\mathrm{CFCl_3}$			Lower BC
52	CF2Cl2	34056	$\mathrm{CF_2Cl_2}$			Lower BC
53	MeBr	34057	$\mathrm{CH_3Br}$			Lower BC
54	N	34058	N			
55	O(3P)	34059	$\mathrm{O(^3P)}$			
56	MACRO2	34060	peroxy radicals			
57	H2	34070	$\mathrm{H_2}$			Lower BC
58	H	34080	H			
59	OH	34081	OH			
60	HO2	34082	$\mathrm{HO_2}$		Yes	
61	MeOO	34083	$\mathrm{CH_3O_2}$		Yes	
62	EtOO	34084	$\mathrm{C_2H_5O_2}$			
63	MeCO3	34085	$\mathrm{CH_3COO_2}$			
64	n-PrOO	34086	$\mathrm{n\text{-}C_2H_7O_2}$			
65	i-PrOO	34087	$\mathrm{i\text{-}C_2H_7O_2}$			
66	EtCO3	34088	$\mathrm{CH_3COO_2}$			
67	MeCOCH2OO	34089	$\mathrm{CH_3COCH_2OO}$			
68	MeOH	34090	CH_3OH			Emitted
69	Lumped N	34098				
70	Lumped Br	34099				
71	Lumped Cl	34100				
72	PASSIVE O3	34149	Passive O3			
73	AGE OF AIR	34150	Age of Air			
74	O(1D)	34151	O(1D)	Yes		
75	NO2	34153	$\mathrm{NO_2}$	Yes		
76	BrO	34154	BrO			

Table 9: Advected tracers treated by CheST (continued)

	STASH name	STASH	UKCA Species	Dry	Wet	Emitted/Lower BC
77	HCl	34155	HCl		Yes	

4.6 Heterogeneous chemistry for the troposphere

This heterogenous chemistry scheme is only available when using the chemistries solved by the Newton-Raphson method and when the GLOMAP-mode aerosol scheme is called to provide aerosol area estimates. The heterogeneous chemistry is controlled by the logical L_UKCA_TROPHET. The scheme considers two reactions: the conversion of N_2O_5 to nitric acid and the self reaction of HO_2 on surfaces (reactions 3 and 4).

The reaction coefficient of the species which is adsorbed on an aerosol surface (k) is (Dentener (1993)):

$$k = (\frac{r}{D_g} + \frac{4}{\nu \times \gamma})^{-1} \times A, \tag{1}$$

where r is the aerosol radius $[cm]$, D_g is the gas-phase diffusion coefficient $[cm^2\ s^{-1}]$, ν the mean molecular speed $[cm\ s^{-1}]$, and γ is the reaction probability [non-dimensional]. A is the aerosol surface concentration in units of $[cm^2\ cm^{-3}]$, calculated as an integral over the log normal distribution using the wet radius calculated in GLOMAP-mode. The gas-phase molecular diffusion coefficient may be calculated from (Bauer et al. (2004)):

$$D_g = \frac{3}{8Ld_q^2\rho_a}\sqrt{\frac{RTm_a}{2\pi}\left(\frac{m_a + m_q}{m_q}\right)}, \tag{2}$$

where L is Avogadros constant, d_q is the diameter of the gas molecule ($\approx 4.5 \times 10^{-10} m$), rho_a is the air density, R the gas constant, T the temperature, and m_a and m_q are the molecular weights for air and the gas.

Two tropospheric heterogeneous reactions on aerosol are considered here:

$$N_2O_5 \Rightarrow 2\ HNO_3, \tag{3}$$

and

$$HO_2 \Rightarrow 0.5\ H_2O_2. \tag{4}$$

Equation 4 represents the self reaction of HO_2 on aerosol surfaces, and a more sophisticated approach is described by Thornton et al. (2008). This approach takes into account the aqueous reaction on the aerosol, but really requires the pH to be estimated.

Both N_2O_5 and HO_2 have uptake coefficients which are estimated for aerosol surfaces composed of sulphate, black carbon, organic carbon, sea-salt, and dust. Secondary organic aerosol is assumed to behave in the same way as organic carbon.

The reaction probabilities for N_2O_5 ($\gamma_{N_2O_5}$) are estimated using the equations outlined in Evans and Jacob (2005), although those for dust have been increased by an order of magnitude following the results of Mogili et al. (2006). For reaction on sea-salt, $\gamma_{N_2O_5} = RH \times 0.0005$ following Thornton and Abbatt (2005). The reaction probabilities for HO_2 (γ_{HO_2}) are estimated for the same surfaces using a variety of sources which have been summarised in Mao et al. (2010).

In the GLOMAP-mode aerosol model, the aerosol surface area concentration for each aerosol mode is calculated from the aerosol number concentration and the wet diameter for each mode, together with the appropriate geometric standard deviation. The heterogeneous rate coefficients are calculated using equation 1 using the aerosol surface area and wet radius from GLOMAP-mode. These rates are then stored in the atmosphere dump and read in so that the chemical solver can use them in the next timestep. This is done because GLOMAP-mode is called after the chemistry.

5 Aerosol Chemistry

Chemical schemes which produce aerosol products have been developed for tropospheric and stratospheric conditions. The sulphur oxidation in these schemes include a gas-phase H_2SO_4 tracer which is produced by the gas-phase $SO_2 + OH \rightarrow H_2SO4 + HO_2$ reaction. As there is no explicit in-cloud sulphate tracer in GLOMAP-mode, the aqueous-phase reactions producing sulphate have no explicit product. Instead, the reaction fluxes are passed into GLOMAP-mode and are used to update the accumulation and coarse mode sulphate mass.

5.1 Tropospheric aerosol chemistry for Newton-Raphson solver

5.1.1 Gas and Aqueous phase Chemistry

The gas and aqueous phase reactions of $SO_2, DMS, CS_2, H_2S, COS$, and monoterpene are shown in table 10. All the species in this table are held as tracers in the model (see table 11). There is currently no ammonium nitrate scheme, but an ammonia tracer is already included.

The incorporation of a soluble species into cloud droplets is quite rapid, and an equilibrium approach is adopted here. This approach is justified by the rapid approach to equilibrium for cloud droplets (Warneck (2000)). Gas to liquid phase equilibrium is described by Henry's law written in the form:

$$C_s \approx [s] = K_H p, \tag{5}$$

where C$_s$ is the molar concentration in mol/l [of cloud water], [s] is the concentration in mol/kg, and p is the gas phase partial pressure in atmospheres, giving the units of the Henry's law constant, K_H, as mol l^{-1} atm^{-1}. The total concentration of the species (C_t) is therefore composed of the sum:

$$C_t = C_s.L + C_g, \tag{6}$$

where C_g is the gas phase concentration in mol/l [of air], and L is the non-dimensional volume ratio for liquid water, calculated from:

$$L = \frac{q_{cl} P M_a}{R T \rho_w}, \tag{7}$$

where q$_{cl}$ is the cloud liquid water content in kg (water)/ kg (air), P the pressure, M$_a$ is the molecular weight of air, T temperature, and ρ_w is the density of water.

Using the gas law and equation(5), the gas and aqueous phase concentrations are related by:

$$C_s = \frac{C_g \times 10^3 K_H R T}{P_0} \tag{8}$$

where P_0 is equal to 1.013×10^3, and the factor of 10^3 converts from mol/l to mol/m^{-3}. Combining equations 6 and 8 gives the aqueous fraction, f$_{aq}$:

$$f_{aq} = \frac{1}{1 + \frac{P_0}{R_g T K_H L \times 10^3}} \tag{9}$$

This is the aqueous fraction for a grid cell entirely in-cloud.

Some of the gaseous species dissolved in clouds (e.g. HNO_3, O_3, H_2O_2, NH_3, and SO_2) are subject to aqueous phase equilibrium, for example:

$$\begin{aligned} H_2O &\rightleftharpoons H^+ + OH^- &(10)\\ HNO_3 &\rightleftharpoons H^+ + NO_3^- &(11)\\ SO_2 &\rightleftharpoons H^+ + HSO_3^- &(12)\\ HSO_3^- &\rightleftharpoons H^+ + SO_3^{2-} &(13)\\ NH_3 &\rightleftharpoons OH^- + NH_4^+ &(14)\end{aligned}$$

The dissociation of dissolved species such as SO_2 means that these species are more soluble than the equilibrium Henry's law constant suggests. This is taken into account by using an effective constant which for SO_2 is related to K_H by:

$$K_{Heff} = K_H(1 + \frac{k_G}{[H^+]} + \frac{k_G k_H}{[H^+]^2}), \tag{15}$$

where k_G and k_H are the equilibrium constants for the aqueous phase dissociation equations shown above. The last term in this equation is negligible. The hydrogen ion concentration (H^+) is currently set as a global number in UKCA.

The routine UKCA_FRACDISS calculates the fractional dissociation of soluble species using the Henry law coefficients held in the chemistry module. Note that the dimension of the henry_defs array is (6,jpdw), so the soluble and wet deposited species must be made identical. For species that do not dissociate, the first two components of the henry_defs array hold the K_{298} and the $\Delta H/R$ values for gas to aqueous transfer. For species with one dissociation position 3 and 4 hold these coefficients for the first dissociation, and for SO_2 only, positions 5 and 6 hold the coefficients for the second dissociation.

Once the dissolved fractions have been calculated, the aqueous-phase reactions are treated as in Berglen et al. (2004), where a rate coefficient appropriate to the total SO_2 is calculated depending on the dissolved fraction, the cloud fraction, and the cloud liquid water. The aqueous-phase reactions are specified in the chemistry modules as (for example): rath_t('SO2 ','O3 ','NULL1 '......), and this equation is identified in the routine ASAD_HETERO, and an appropriate rate coefficient calculated for the cloudy parts of the model.

5.2 Tropospheric aerosol chemistry for Backward-Euler solver

The aerosol chemistry currently treats the degradation of SO_2, DMS, NH_3, and monoterpene. SO_2 is oxidised by OH and by H_2O_2 and O_3 in cloud droplets.

5.2.1 Chemical scheme

The chemistry for the backward-Euler scheme is similar to that used for the Newton-Raphson scheme in section 5.1, but only SO_2, DMS, and Monoterpene are treated. In addition, the aqueous-phase chemistry of SO_2 oxidation contains only the HSO_3^- + H_2O_2(aq) and SO_3^{--} + O_3(aq) reactions which take the rate coefficients given by Bower et al. (1991). These aqueous-phase reactions are converted into equivalent gas-phase processes following Berglen et al. (2004). The other main difference is that the DMS oxidation scheme is parameterised as described below. The oxidation of ammonia by OH is included, but NH_3 does not participate in aerosol production.

5.2.2 Parameterisation for DMS oxidation

This analysis of DMS oxidation has been constructed on the basis that the lifetimes of intermediate species between DMS and the final products are insignificant, i.e. that the distribution of the final products depends only on DMS and oxidant concentrations. In this version of the scheme the reaction of DMS with NO_3 has been included, as it is intended to be used in UKCA where this oxidant is already available.

This scheme is mainly based on the work of Jenkin (1996) and Koga and Tanaka (1999). Figure 5.2.2 shows the scheme used. The main simplification is that all the oxidation of DMS proceeds to CH_3SO_2, with no intermediate species. Full details of the scheme used in UKCA are given in tables 12 and 13

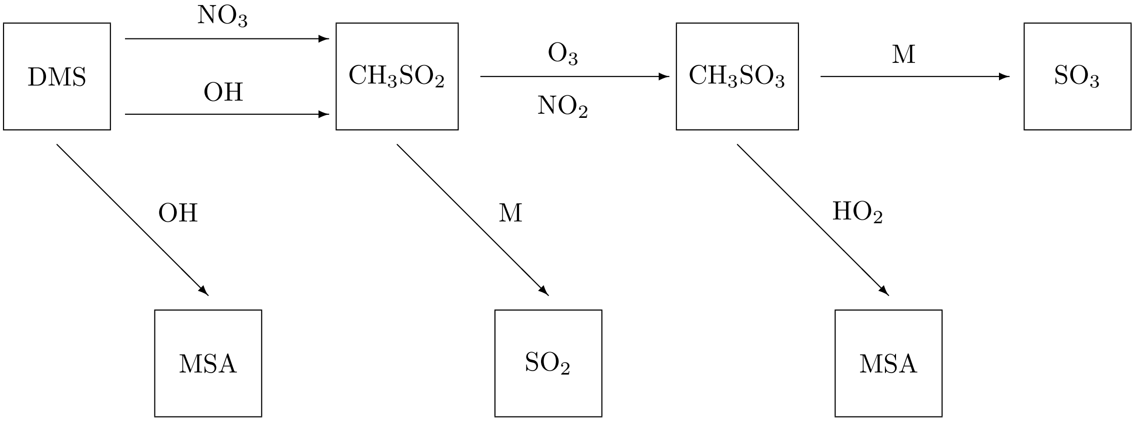

Figure 1: Simplified DMS oxidation scheme.

5.3 Stratospheric aerosol chemistry

Several of the GLOMAP-mode routines have been adapted to be applicable in both tropospheric and stratospheric conditions, and these changes are described in section 13.3.10 and Emmerson et al., (2012, in prep.). This stratosphere-troposphere version of GLOMAP-mode requires to be driven by a sulphur chemistry scheme, so the UKCA standard stratospheric chemistry scheme (also known as CheS) was extended to also include a sulphur chemistry scheme appropriate for the stratosphere. The tracers for this “stratospheric aerosol chemistry” are those in Table 11, but without DMSO, MSA, NH_3, Monoterpene, and secondary organic, together with an extra tracer for SO_3. The gas phase reaction scheme follows Weisenstein et al. (1997) and SPARC (2006) including thermal and photolytic reactions for COS, SO_2, SO_3, and H_2SO_4, see table 14. Reactions of H_2S, CS_2, and DMS with $O(^3P)$ are also included. The tropospheric species and reactions are similar to the tropospheric aerosol chemistry (see table 10), with DMSO and MSA not included as products.

6 Chemical Solvers

Two chemical solvers are used in UKCA. Some of the tropospheric chemistry schemes currently use an explicit backward-Euler solver, but the stratospheric chemistry schemes and the parameterised isoprene scheme use the ASAD system with a Newton-Raphson (N-R) solver. This solver performs well, but is not currently well load balanced on the IBM computers.

6.1 ASAD Framework

ASAD is a chemical solver system (Carver et al. (1997)) designed to run various chemical solvers from files containing details of the chemical species, rate coefficients, and deposition rates. A strength of this system is that it will solve any consistent chemical system without modification. The implementation of ASAD in UKCA contains changes to the ASAD system used elsewhere. The available chemical solvers are: 1) Newton-Raphson solver; 2) Implicit Backward-Euler solver, and 3) the IMPACT solver Carver and Stott (2000)) for family chemistry. Family chemistry is not currently used by UKCA, and the only ASAD solver in routine use in UKCA is the Newton-Raphson.

The Newton-Raphson solver is derived from that used by Wild and Prather (2000), and has been used for the stratospheric chemistry Morgenstern et al. (2009) with a one hour chemical timestep. This solver employs an interative technique which will currently inhibit bit comparability of the chemistry across different processor configurations as the solver is supplied with a two-dimensional array representing a horizontal surface. The derivative of any steady-state species with respect to ozone is included in the calculation of the sparse Jacobian array. Explicit code for each steady-state species is required, and currently only O(1D), O(3P), N and H may be set as a steady-state species.

To enable source code version control, the external files used by the ASAD system have been replaced by a series of structures contained in (or referenced by) the module UKCA_CHEM1_DAT. The arrays required by ASAD are selected by a call to UKCA_CHEM1_INIT contained in this module, depending on the chemical scheme chosen. At this stage a check on dimensions of the various structures is made. To allow the ASAD system to be configured to different resolutions, allocatable arrays are defined in the module ASAD_MOD. These replace the arrays originally defined in common blocks in various header files. The structures used by ASAD to define the chemistry are defined below. As well as the definitions of the rate coefficients contained in these structures, exceptions to the normal rate laws are handled explicitly in the routines ASAD_BIMOL and ASAD_TRIMOL. For the bimolecular equations, these include the pressure term in the OH + CO reaction, branching ratios of reactions such as OH + C_3H_8, and the OH + $HONO_2$ rate, together with the water vapour correction term in the HO_2 + HO_2 reaction.

6.2 Backward-Euler solver

Some tropospheric chemistry schemes are currently solved using an explicit backward-Euler solver based on Hertel et al. (1993). This calculates the production and loss terms and solves directly, within an iteration loop. This method was initially used because it was found to vectorise well, and it is bit comparable across processor configurations. Another advantage is that short-lived species do not need to be advected. Currently the non-advected species are initialised and stored in the dump, as this has been found to improve solver accuracy. Each tropospheric chemistry scheme has two routines in UKCA which are scheme dependent. For example, the standard tropospheric chemistry scheme has a solver (UKCA_DERIV) and a rate coefficient routine (UKCA_CHEMCO).

The default value of the B-E timestep is 300s and the default number of iterations is 8. It is possible to change the scheme from using these default values by setting the values dts0 and nit in the run_ukca namelist.

6.3 Driving the solvers from UKCA

The dimensions of the chemical components are set inside the code (in subroutine ukca_setup_chem) depending on the value of the namelist variable i_ukca_chem. Table 15 shows the chemical array dimensions. These available from the UKCA module called ukca_option_mod. Logical variables defining the chemical scheme are also held in this namelist. These logical variables are also set in ukca_setup_chem depending on the value of i_ukca_chem.

6.4 Chemical definition arrays

There are five arrays which define the chemistry used by the ASAD solvers: Each array consists of a structure defining the elements required.

- **chch_defs** array - this defines the tracers, steady-state, and constant species, and also defines which species are active in the dry deposition, wet deposition, and emission schemes.
- **ratb_defs** - this array defines the bimolecular reactions and rate coefficients
- **ratt_defs** - this array defines the termolecular reactions and rate coefficients
- **ratj_defs** - this array defines the photolysis reactions and the filenames
- **rath_defs** - this array defines the heterogeneous reactions
- **depvel_defs** - this array defines the dry deposition velocity used when the interactive scheme is switched off. The dry deposition velocity is defined for five different surfaces (water, forest, grass/shrub, desert, and snow/ice) and six different times (day, night, average for summer and winter).
- **henry_defs** - this array defines the Henry law coefficients for the species involved in wet deposition.

The subroutine UKCA_CHEM1_INIT (contained in CHEM1_DAT) fills these arrays from arrays defined for each chemical scheme. The length of each array is checked against the sizes set in ukca_setup_chem, for example the chch_defs array should have a length of jpspec.

The order of tracers and species in the chch_defs, depvel_defs, and henry_defs arrays must be internally consistent. For example, the order of entries in henry_defs must match the order of species which are active in wet deposition according to chch_defs. Likewise, the order of deposition velocity entries in depvel_defs must match the order of species which are dry deposited in the chch_defs array. However, there is no need for the order of tracers in chch_defs to match that in the STASHMASTER file or the nm_spec array (the STASHMASTER and the nm_spec array themselves also need to be internally consistent). UKCA tracers extracted from the D1 secondary store are automatically placed in the correct order to match that of chch_defs using the nm_spec array defined in UKCA_SETD1DEFS routine.

6.5 Initialisation of chemical species

In the chch_defs file, species are labelled as 'TR' (tracers), 'SS' (Steady-state species), 'CT' (constant value), or 'CF' (constant field). Species labelled as tracers are set from the tracer array, while steady-state species are initialised to a small number. Constant species like CO_2 are set to a global constant in routine UKCA_MAIN1. Only CO_2, H_2, N_2, O_2, and CH_4 may be set in this routine, and other species labelled as 'CT' will be set to zero in ASAD_FYINIT, and a warning message issued. Currently the only species which may be set to a constant field is water vapour and this is set to model water vapour in routine ASAD_INICNT. This is only required if water vapour is not selected as a tracer, otherwise the water vapour tracer is filled from model water vapour in UKCA_MAIN1. If feedback from UKCA to model water vapour is required, the flag 'L_ukca_h2o_feedback' may be selected to set model water vapour to the UKCA tracer after the chemistry.

Prognostic variables in the MetUM (such as tracers) are initialised at the start of the model run by the reconfiguration which provides the start dump. The prognostic data in the start dump may come from a number of alternative sources. The simplest case is where the required field(s) are present in the source dump used as input to the reconfiguration program. In this case the user does not need to take any special action. If the source data does not include one or more prognostics, the user needs to provide information on how to initialise the data in the start dump. This is done using the items namelist in the reconfiguration namespace. Options for initialisation include giving the field a constant value or using an ancillary file as the source of data.

7 Photolysis

Three schemes may be selected: a scheme based on the interpolation of tabulated values (2D photolysis), and two different versions of the online Fast-J scheme. The code currently contains both the original Fast-J scheme (Wild et al. (2000) which is only suitable for the troposphere and also Fast-JX (Neu et al. (2007), Prather (2012)) which has an extended wavelength range suitable for stratospheric conditions. The choice of scheme is set in the main UKCA namespace in rose edit.

A comparison of the 2D photolysis rates and Fast-JX in a Chemistry Transport Model may be found in Voulgarakis et al. (2009).

The namelist integer i_ukca_photol selects which photolysis scheme to use. See Table 16 shows the values of this integer for each photolysis scheme.

7.1 2D photolysis scheme

If this scheme is selected, tropospheric photolysis rates are interpolated using results from the Cambridge 2D model (Law and Pyle (1993)). These are stored at five day intervals with three times of day. The rates are interpolated in time and location. For the stratospheric chemistry schemes, selecting the 2D photolysis scheme indicates that the model will use photolysis rates calculated from UV fluxes and the appropriate cross sections. For some species, the two photolysis rates for the stratosphere and troposphere are interpolated in height, with tropospheric rates used below 300 hPa, and stratospheric rates above 200 hPa. When using this scheme the location of the input files can be specified using rose edit. Also note that this scheme by default uses binary input files which can be prepared from Fortran program make_binary.f90 which is in the UM repository along with the ASCII source data sets at `AUX/trunk/ctldata/UKCA/tropdata/photol`. Unlike most MetUM binary files, these need to have the same endianess as the computer system being used so may need to be regenerated if there is a change of platform. The program check_binary.f can be used to check if the code can be read in correctly on your system.

7.2 Fast-J and Fast-JX photolysis schemes

7.2.1 Fast-J

Fast-J is currently being used by an operational model configuration and so remains in use at present. However, Fast-JX should be used for all new model configurations as it is more efficient and Fast-J will be retired once the operational models have been tested properly with Fast-JX.

Fast-J (Wild et al. (2000)) is a flexible and accurate photolysis scheme, which calculates photolysis rates in the presence of an arbitrary mix of cloud and aerosol layers. The algorithm is sufficiently fast to allow the scheme to be incorporated into 3-D global chemical transport models and have photolysis rates updated hourly. It enables tropospheric chemistry simulations to include directly the physical properties of the scattering and absorbing particles in the column, including the full, untruncated scattering phase function and the total, uncorrected optical depth. The scheme has a 7-bin quadrature covering wavelengths from 291 to 850 nm.

As implemented in the MetUM at the current time, it uses data from the Unified Model for sulphate aerosol, liquid and ice cloud water content and ozone. These are turned into optical depths in the interface routine ukca_fastj.F90.

Fast-J can be turned on from Rose by using the corresponding switch on the UKCA namespace and the location and name of the file containing cross section data (normally jv_spec.dat) can be set here. A copy of this file is stored in the AUX project at `AUX/trunk/ctldata/UKCA/tropdata/fastj`

7.2.2 Fast-JX

The Fast-J photolysis scheme was extended by Bian and Prather (2002) to Fast-J2, making use of 18 bins to cover the wavelength range from 177 to 291 nm. This made Fast-J2 suitable for implementation in stratospheric chemistry models. Fast-JX was a further update: scattering is calculated for all 8/12/18 wavelength bands instead of scattering in the UV bands being treated as pseudo absorption (which produced problems in the winter stratosphere). There are also technical differences (code optimised especially for vectorisation) and an improvement to the calculation of extra layers for optically dense levels. The Fast-JX version currently in the Unified Model is version 6.5 which was released in September 2009.

Fast-JX can also be turned on using the switch on the UKCA namespace, and the location and name of the file containing cross section data and data on scatterers can be set here. A copy of these files are stored in the AUX project at `AUX/trunk/ctldata/UKCA/tropdata/fastj`. If using Fast-JX, there are several additional options. It is possible to choose 8, 12 or 18 wavelength bins. The 18 wavelength version is the full Fast-JX version, choosing 12 is only suitable for troposphere only models and drops cross sections for stratospheric species, the 8 bin version is a fast troposphere-only version. The choice between the 8 and 12 bin versions is a trade off between accuracy and speed.

Fast-JX has a lower wavelength limit of 177nm, which doesn't cover all the reactions in upper parts of the atmosphere. To cope with this, three options are available above a cut-off pressure level chosen with rose edit (typically 20 Pa). The first option is to use stratospheric photolysis rates based on the look up table approach of Lary and Pyle (1991) with updated cross section measurements (Morgenstern et al. (2009)) for the wavelengths below 177nm and use the Fast-JX rates for the longer wavelengths. The second option is to just use the look up table rates and the final option is to use Fast-JX only.

As in Fast-J the sulphate field from the troposphere is used. Currently, this sulphate field is from the CLASSIC aerosol scheme, the predecessor to GLOMAP-mode. It is also possible to use a pre-defined reference sulphate aerosol file in the stratosphere.

8 Dry deposition

Two schemes are available: a scheme based on specified dry deposition velocities for each species involved, and a scheme which depends on predicted resistances from the conditions at each point (called the *interactive dry deposition scheme*). The first scheme is used when the interactive scheme is turned off.

8.1 Interactive dry deposition scheme

This scheme calculates the dry deposition rates using a resistance-based approach, where the deposition velocity, v_d, is calculated by:

$$v_d = 1/(r_a + r_b + r_c),$$

where r_a is the aerodynamic resistance, r_b is the quasi-laminar sublayer resistance, and r_c represents the bulk surface resistance. The treatment follows that of Wesely (1989). Calculations are carried out using the surface tile scheme, so that both the physical and vegetation characteristics can be taken into account. The nine tile types are defined as: Broadleaved trees, Needleleaf trees, C3 Grass, C4 Grass, Shrub, Urban, Water, Bare Soil, and Ice.

The aerodynamic resistance (r_a) is calculated from the wind profile taking into account atmospheric stability and the surface roughness:

$$r_a = (ln(z/z_0) - \psi)/(ku_*),$$

where z_0 is the roughness length, ψ is the Businger dimensionless stability function, k is von Karman's constant, and u_* is the friction velocity.

The quasi-laminar sub-layer resistance is calculated from:

$$r_b = (S_c/P_r)^{2/3}/(ku_*),$$

with S_c the Schmidt number, and P_r the Prandtl number.

Table 17 shows the species covered by the interactive scheme.

The scheme that calculates surface resistances to land and the vegetation is too complex to describe in detail, as the details depend on the surface type and the chemical species. The surface resistance for each of the nine tiles is specified for each chemical species. Stomatal resistances are calculated for O_3, NO_2, PAN, SO_2, and NH_3. These resistances are then combined, and the contributions from each tile type are combined.

The interactive dry deposition scheme is selected by chosing the option: "UKCA interactive dry deposition scheme".

8.2 Deposition velocity scheme

This scheme uses the tabulated dry deposition velocities for the surface. The type of surface used is selected by the roughness length and the sea-ice cover. The dry deposition velocities are specified for the following surface types: water; snow/ice; forest; grass/shrub; and desert. Values are provided for day and night conditions, and are also specified as an average over the entire day. The average value is unused in UKCA. This scheme is the default dry deposition scheme and is used if the interactive scheme is not selected.

9 Wet deposition

The wet deposition scheme for the tropospheric gas-phase species is that implemented and validated in the TOMCAT CTM (Giannakopoulos (1998) and Giannakopoulos et al. (1999)).

Wet deposition rates are parameterised as first order loss rates, calculated as a function of the modelled convective and large-scale precipitation. The removal rates are also a function of the effective Henry's Law co-efficient for each species which takes the effects of dissociation and complex formation on a species' solubility into account.

Which species are wet deposited depends on the chemistry scheme being run. See the tables for each scheme in section 4 for more information.

Each scheme has a module ukca_chem_xxxxx.F90 in which the array chch_defs_xxxxx controls which species are wet deposited and henry_defs_xxxxx holds the coefficients used to calculate the effective Henry's Law co-efficients.

10 Emissions

The emission inputs to UKCA can be broadly classified into two categories: *Offline* which are pre-computed fluxes read in from ancillary files; and *Online* which are computed in realtime during the simulation making use of online meteorological variables from the UM. Examples of online emissions currently in UKCA are lightning NOx, sea-salt (from GLOMAP-mode) and wetland methane emissions (from Land Surface section).

A comprehensive list of all the emission species required by each UKCA Scheme is given in Table 18. Note that the units specified for the offline species refer to the values as stored in the ancillaries. Similarly, those for online species refer to the quantities as first computed by the relevant routines, before being accessed/ processed by UKCA.

The offline emissions for UKCA have to be read in through the "User Ancillary" route of the UM. Currently, only one I/O stream each is available for the user single-level and multi-level ancillaries. This implies that all the emission species for a particular type (surface or multi-level) have to be stored in a single file and updated with the same time frequency. Similar to the other UM ancillaries used to update fields, the emission ancillaries can either hold data as a timeseries (covering the whole simulation period) or as a cyclic/ 'periodic' set (e.g. 12 monthly fields with an unspecified year stamp).

The emission species used by each UKCA scheme are defined through the *em_spec* array in the UKCA_SETD1DEFS routine.

10.1 Surface emissions

The surface emission fields are read in through the 'User Single-level Ancillary' route.

There are 20 slots available for surface emissions (Sec:0 item:301-320) in the STASH. Note that these items are not defined in the STASHmaster and the required species/ items have to be 'switched on' through a userSTASHmaster file. The emission ancillary files themselves must contain the same item code in LOOKUP header of the fields.

The Aerosol Chemistry, used in conjunction with the UKCA schemes (currently not available for RAQ Chem), requires emissions for precursors of sulphate and secondary organic aerosols, while GLOMAP-mode (if used in the H2SO4, Nacl, BC, OC 5-mode setup), additionally requires emissions for carbonaceous aerosols. TropIsop and Strat+Trop Schemes with Aerosol Chemistry require NVOC emissions, which are essentially represented as CH_3OH in the model.

For stratospheric configurations (Strat, Strat+Trop), the offline as well as online CH_4 emissions may be overwritten by CH_4 lower boundary conditions as controlled through the `I_UKCA_SCENARIO` integer.

As seen in Table 18, Stratospheric Chemistry only requires a subsection of the surface emissions. However, for the sake of convenience and to maintain uniformity, by default the StratChem jobs use the same emission userSTASHmaster file and ancillary as the other (non-RAQ) Chemistry jobs. This is also true for surface BC/OC emissions required by GLOMAP-mode, as they may be specified and read in for all aerosol chemistry configurations, irrespective of whether GLOMAP-mode is active or inactive.

Note that the S-cycle emissions (SO_2,DMS,NH3) required for aerosol chemistry currently have to be read in through the CLASSIC Aerosol scheme and are accessed by UKCA via D1. This implies that the CLASSIC S-cycle component needs to be switched ON when AeroChem is required. CLASSIC is activated via the namespace: Section 17 - Aerosol (Classic, dust and murk)

The SO_2 'High-level' emission from Industrial fuel, forest fires, shipping, etc is actually a single-level field which is then added to the appropriate user-defined level (normally $\approx$ 1 km height) in the 3-D SO_2 array.

The limitation (for User Ancillaries) of having a common time frequency for all species makes it difficult to provide emissions with any short-term (diurnal, weekly) variations. These variations in emissions are especially critical for Air quality applications. To partly overcome this limitation, the RAQ based Air Quality UM configuration applies a pseudo diurnal profile to all the emissions through a UM branch, while the TropIsop and the Strat+Trop UKCA schemes currently apply such a diurnal profile only to isoprene (routine UKCA_DIURNAL_ISOP_EMS). This routine makes use of the solar zenith angle and latitude to compute the expected number of sunshine hours and spreads the daily total isoprene emissions over this period.

The surface emissions, after conversion to appropriate units are added to the UKCA tracers by calling the UM routine TR_MIX which accounts for the boundary-layer mixing of the surface quantity.

The online surface emissions used by UKCA include the interactive wetland methane emissions and sea-salt emissions. The wetland CH4 emissions are optional for UKCA, but must be selected if the surface emissions ancillary does not contain a contribution from wetlands. These are computed by the Wetland Emissions model (Gedney et al. (2004)) as a diagnostic in the Land Surface/ Hydrology component of the UM using water table depth/ wetland fraction, soil carbon content and soil temperature. The diagnostic (8-242) is then read in from D1 by UKCA and converted to kg(CH4)/m^2/s before being added to the CH4 tracer. *Note that these emissions have not been extensively tested with recent UM versions and users should seek advice before using this option in their simulations.* Note that methane emissions are unused by the model when prescribed surface methane concentrations are used. See section 16.

The sea-salt emissions are computed in GLOMAP-mode (routine UKCA_PRIM_SS) as bin-resolved sea-salt emission fluxes from a size-resolved sea-spray source function of Gong (2003), basically as particles/gridcell/s and are then directly added to the appropriate soluble accumulation and coarse modes.

10.2 Lightning NO_x Emission

The production of NO_x through thermal dissociation of O_2 by lightning is computed at real-time in UKCA (routines: UKCA_LIGHT, UKCA_LIGHT_CTL) based on methodology originally implemented in the Cambridge TOMCAT model. This method makes use of parametrised lightning flash frequency (Price and Rind (1992)) of 3.44 x $10^{-5}H^{4.9}$ per min over land, and 6.4 x $10^{-4}H^{1.73}$ per min over ocean (H=cloud depth in km), along with a Cloud-Cloud and Cloud-Ground flash ratio based on the grid-cell latitude (Price and Rind (1993)). Price and Rind (1994) derived a *spatial calibration factor* c=0.97241exp(0.048203R), where R=(latidude resolution x longitude resolution), both in degrees, which renders lightning flash rates independent of model resolution. A minimum cloud depth of 5 km is required for the lightning NO_x to be activated. The cloud depth is determined using the convective cloud bottom and top levels diagnostics (Sec5:218,219) from the UM Convection Scheme. The lightning NO_x is initially produced as 3-D, kg(NO2)/gridcell/s and later converted to kg(NO)/kg(air)/s before being added to the NO tracer.

10.3 Other 3-D emissions

The offline 3-Dimensional emissions required by UKCA includes the NO_x emissions from aircraft for all UKCA schemes, SO_2 volcanic emissions for Aerosol Chemistry and the BC, OC emissions from biomass burning for GLOMAP-mode.

The aircraft NO_x and BC/OC emissions are input through the User Multi-level ancillary route. The STASH slots of Section 0, item 321-340 are available for this purpose, and similar to the Single-level ancillary, have to be switched ON through userSTASHmaster files.

The aircraft NO_x emissions are read in as kg(NO2)/gridbox/s before being converted to kg(NO)/m^2/s and added to the NO tracer.

The SO_2 volcanic emissions (as 3D natural emissions), similar to the surface SO_2 emissions, are accessed by UKCA through CLASSIC

The emissions are read in as kg(S)/(m^2 s) and converted to kg (SO2)/(m^2 s) before being combined with the SO_2 'high-level' emissions and added to SO_2 tracer.

The biomass burning BC and OC emissions for GLOMAP-mode are read in as kg(C)/m^2/s before being converted to kg(C)/gridcell/s and added appropriately to the Aitken soluble and insoluble modes. (routine: UKCA_PRIM_CAR).

11 New NetCDF emission system

11.1 Introduction

In the current emission code of UKCA, 2-dimensional (2-D) surface and 3-dimensional (3-D) emissions are read by the model as user single- and multi-level ancillary files, respectively. The routine UKCA_SETD1DEFS sets the number of chemical tracers with surface (n_chem_emissions) and 3-D emissions (n_3d_emissions) as well as the number of emitted fields in the GLOMAP-mode aerosol scheme (n_MODE_emissions) and the number of dust bins (n_dust_emissions) for any given chemistry scheme. The array em_chem_spec includes the list of surface and 3-D emissions used in the chemistry scheme. Emission diagnostics are output in Section 0, for which user STASH-Master files are needed. One of the main limitations of the code is the impossibility of treating emissions from independent source sectors separately.

The new UKCA emission code lodged at UM vn8.6 introduces a number of enhancements:

- Input emission files are NetCDF instead of in ancillary format.
- Introduce flexibility and allow the use of different emission fields to account for independent source sectors for any given tracer.
- Avoid as much as possible any inconsistencies in the units of the emission fields, by setting them through metadata attributes in the NetCDF files and carrying cross-checking within the UKCA code.
- Improved handling of emissions. The values of all gas phase emission fields are stored in an 'emissions' structure, and then they are added to the corresponding tracers over all model levels via call to TRSRCE and TR_MIX; note that this second routine also does boundary layer tracer mixing of tracers. The only exception to this are the emissions of sulfur dioxide (SO_2) from explosive volcanic eruptions, which are occasionally injected in the stratosphere and are not present in all chemistry schemes of UKCA; they are treated separately from the rest of the emission fields in this code.

At present the new emission code only works for emissions of gas phase species and cannot be used with GLOMAP-mode aerosol configurations of UKCA. In the medium term this code will coexist with the current emission code of UKCA. The logical switch L_ukca_new_emiss has been introduced for that purpose. When it is set to .TRUE. then UKCA_MAIN1 will call the new routine UKCA_NEW_EMISS_CTL, otherwise UKCA_EMISSION_CTL will still be used.

11.2 Description of the code

Among others, the new emission code consists of the following routines. All of them are included in modules even if not stated below:

1. UKCA_NEW_EMISS_CTL. Top-level subroutine for the new emission system. It is expected to replace UKCA_EMISSION_CTL in the long term. The code flow within this routine will be described in Section 11.3 once the other main subroutines/modules relevant to the new UKCA emission system have been introduced.

2. UKCA_EMISS_MOD. Module containing a number of procedures whose main aim is to allocate, set-up and update an emissions data structure holding information on the emission fields. This data structure is declared as follows at the beginning of the module:

```
! Emission Data structure
TYPE ukca_em_struct
  CHARACTER (LEN=256) :: file_name
  CHARACTER (LEN=80)  :: var_name
  CHARACTER (LEN=10)  :: tracer_name
  CHARACTER (LEN=256) :: std_name
  CHARACTER (LEN=256) :: lng_name
  CHARACTER (LEN=30)  :: units
  INTEGER             :: update_freq
  INTEGER             :: update_type
  LOGICAL             :: l_update
  LOGICAL             :: three_dim
  REAL                :: base_fact
  REAL, POINTER       :: vert_scaling_3d (:,:,:)
  CHARACTER (LEN=20)  :: hourly_fact
  CHARACTER (LEN=20)  :: daily_fact
  CHARACTER (LEN=30)  :: vert_fact
  INTEGER             :: lowest_lev
  INTEGER             :: highest_lev
  REAL, POINTER       :: values (:,:,:)
  REAL, POINTER       :: diags (:,:,:)
END TYPE ukca_em_struct

! Super array of emissions
TYPE (ukca_em_struct), ALLOCATABLE :: emissions (:)
```

See description of all variables in Table 19. Each emission field is first read from NetCDF files or calculated online within the UKCA code (at present this is the case only for NO_x emissions from lightning and CH_4 emissions from wetlands) and then stored as an item in the emissions structure. When an emission field is read from a NetCDF file then some of the variables in the emissions structure will correspond to metadata attributes present in NetCDF files (see Table 21).

This module contains the following main subroutines:

- UKCA_EMISS_INIT. It includes a couple of loops through the NetCDF emission files, which are input to the model through the RUN_UKCA namelist. The first loop identifies the total number of emission fields present in these files (num_cdf_em_flds). Then all the online emissions are considered (for the moment only NO_x from lightning and CH_4 from wetlands if present) to get the total number of emission fields that will be included in the emissions structure (num_em_flds). The emissions structure is then allocated as

```
ALLOCATE (emissions(num_em_flds))
```

and some of the variables in it are initialised to default values via call to UKCA_EM_STRUCT_INIT (subroutine present in the same module). The second loop through the NetCDF emission files has the objective of reading some metadata attributes and information about the dimensions. Both this loop and some additional code for online emissions are then used to allocate/fill some fields in the emission structure. After the call to UKCA_EMISS_INIT each emission field will be stored as a separate item in the emissions structure.

- UKCA_EMISS_UPDATE. At the first time step and when the model time since start corresponds to a full hour this subroutine checks whether each emission field present in the NetCDF files needs to be updated. If so then it calls GET_EMFILE_REC (within the same module) to get the two closest time records in the NetCDF file. Then it calls EM_VAR_CHECK_DIMS to get information on the dimensions and later allocate the arrays with emission values, which are read within the call to EM_GET_DATA (note that these two subroutines are contained in the module EMISS_IO_MOD described below). If the time in a register of the NetCDF file corresponds to the current model time then EM_GET_DATA is called only once, otherwise it is called twice and emission values are interpolated to the model time by using the same subroutine as REPLANCA, i.e. T_INT.
- GET_EMFILE_REC. It calls TIME2SEC to get the current model time in hours and seconds. Then it calculates the target time of the model as fractional hours (fhr_now). Finally it loops over the time records in a given NetCDF file, calling EM_GET_TIME_REC (in module EMISS_IO_MOD), until it finds the two registers which are closest to the current model time. Note that GET_EMFILE_REC includes some conditions needed to interpolate monthly emission fields between December and January when emissions are periodic and the model time is between mid-December and mid-January. When users intend to test a new emission dataset, it is advised to run UM simulations printing extra diagnostic messages and examine the output from this routine to make sure that interpolations are done as expected.

3. EMISS_IO_MOD. Module holding subroutines which call some Fortran NetCDF procedures to get information/values of dimensions/variables present in the NetCDF emission files. It includes a number of subroutines and an interface:

   - EM_FOPEN and EM_FCLOSE. Open and close a NetCDF file.
   - ND_ERROR. Check return status of a NetCDF call. Stop the model if needed by calling EREPORT.
   - EM_GET_VAR_INFO. Used to obtain the following information on a variable whose name or id has been provided: variable id or name, number of dimensions and corresponding sizes, whether it is record/unlimited dimension, and variable type.
   - EM_VAR_CHECK_DIMS. Check that dimensions of a variable in a NetCDF file match global sizes.
   - EM_GET_TIME_REC. Identify the time dimension in a NetCDF file and get the record for the requested time.

- EM_GET_DATA. Interface block used for overloading. A generic call to EM_GET_DATA will identify the type (always real with three dimensions in the present version of the code) of an INTENT(INOUT) argument to select the appropriate subroutine, read the values of the emission field and store them in that INTENT(INOUT) argument.

4. UKCA_EMISS_FACTORS. Module containing four main subroutines to apply conversion factors to the emission values (if needed). The subroutine UKCA_EMISS_INIT (in module UKCA_EMISS_MOD described above) reads the main information about the scaling factors (as character variables) from the attributes present in the NetCDF files. Then such information is passed as input arguments to the subroutines in this module, which then get the appropriate conversion factors. The four subroutines are:

    - VERTICAL_EMISS_FACTORS. It creates a 3-D array holding the factors needed to spread emissions on a number of model layers (if needed) over the model domain. Some average 1-D vertical profiles from the scientific literature have been included for a number of SNAP source sectors in the case of the Regional Air Quality (RAQ) chemistry scheme; when this is the case the subroutine REGRID_VERTIC_PROFS, also present in the same module, is called to convert the average vertical profiles to a 3-D array valid for the given model configuration.
    - HOURLY_EMISS_FACTORS and DAILY_EMISS_FACTORS. They get the appropriate factors to account for hour-to-hour (for hours = 0, ..., 23) and day-to-day (for days Sun=1, Mon=2, ..., Sat=7) variability in the emission fields, respectively. This may be needed because the input NetCDF emission files will often contain monthly average values. The factors will be equal to 1.0 when no conversion is needed. At present only the factors 'traffic_uk' have been included to account for the known diurnal/weekly cycle of emissions over the UK, which is relevant for simulations with the RAQ scheme; additional time profiles for other source sectors are expected to be implemented in the future. Note that implementing a weekly cycle would not have any meaning for jobs with a 360-day calendar; in that case DAILY_EMISS_FACTORS will not be called by UKCA_ADD_EMISS and this routine will make sure that the only daily emission factors allowed (via attributes) in the NetCDF fields are empty or equal to 'none'.
    - BASE_EMISS_FACTORS. It applies some conversions based on the units of the emission fields. If there are special units (e.g. emissions expressed as nitrogen, carbon or sulfur) then the subroutine GET_BASE_SCALING, also present int the same module, is called to get the right conversion factor.

5. UKCA_ADD_EMISS. It goes through all fields in the emissions structure and compares the variable emissions(:)%tracer_name to the list of tracers to identify the position of the 4-D array em_field which corresponds to the emitted tracer. Then emissions(:)%values, multiplied by the corresponding temporal and vertical scaling factors, are added to that position of em_field. Note that this code allows to add several emission fields from different source sectors to the position of em_field that represents a single tracer. Within the same part of the code emission diagnostics are calculated for each emission field and stored as emissions(:)%diags (:,:,:); in the case of 2-D surface emissions such diagnostics are column- integrated and stored as emissions(:)%diags (:,:,1). Then within a loop for all tracers, TRSRCE and TR_MIX are called in this order to add em_field to the corresponding tracer. TRSRCE adds em_field from the second to the top model layer, and then

TR_MIX adds em_field at the lowest model level and also does boundary layer mixing of tracers. Emissions of volcanic SO_2 from explosive volcanic eruptions into the stratosphere are kept separated from the emissions structure; if present they are injected at the very end of this routine via call to UKCA_VOLCANIC_SO2.

6. UKCA_EMISS_DIAGS. Create total emission diagnostics for 2-D and 3-D emission fields. Such diagnostics include all temporal/vertical/unit conversions and in the case of 2-D emissions they have been integrated within the model columns (such calculations are done within UKCA_ADD_EMISS). UKCA_EMISS_DIAGS loops over the list of emitted species present in the array em_chem_spec, identifies whether each element corresponds to a 2-D or 3-D emission, and looks for all values of emissions(:)%tracer_name matching each element in em_chem_spec to add up all the corresponding values of emissions(:)%diags (:,:,:) and calculate a total diagnostic which is stored in the array em_diags (:,:,:). Then that array is passed to the routine UPDATE_EMDIAGSTRUCT, which updates the corresponding fields in the structure emdiags (see notes below).

   Once all fields in the emdiags structure have been updated within the previous loop, UKCA_EMISS_DIAGS prints to STASH each emission diagnostic one by one. For that it gets the corresponding STASH item number through a call to the function GET_EMDIAG_STASH and passes that item as well as the corresponding field in the structure emdiags to the subroutine COPYDIAG, which copies the diagnostics to the array stashwork. COPYDIAG_3D is called instead in the case of 3-D emissions.

   Emission diagnostics are stored in Section 50. At present time only item numbers 156-172 are used, which correspond to the 17 elements present in em_chem_spec for the RAQ chemistry scheme (16 surface emissions and one 3-D emission field for aircraft NO_x). See Table 20. This code will need to be updated to output additional emission diagnostics for any other chemistry scheme, but only those diagnostics which are not present in RAQ should be added to avoid repetition and inconsistencies in the STASH item numbers.

   2-D emission diagnostics are used for surface, high-level and single-level emissions. The calculation of a total 2-D emission diagnostic, including emissions from n source sectors for a given species and integrated over all grid cells from surface to the top of the model for a given lat/lon location, is done as follows:

$$\sum_{i=1}^{n}\sum_{j=1}^{m} E_{ij}(ilon, ilat) \tag{16}$$

   where

```
Eij (ilon,ilat): Emission field (in kg m-2 s-1) of a given species
  for source sector i within a grid cell with ilon, ilat and j
  indices for latitude, longitude and vertical coordinate,
  respectively
n: number of source sectors
m: number of model levels
```

Note that the integration over all model levels above each surface grid cell is done in UKCA_ADD_EMISS while fields from all available source sectors are added in UKCA_EMISS_DIAGS.

The calculation of a total 3-D emission diagnostic is as follows:

$$\sum_{i=1}^{n} E_i(ilon, ilat, iz) \qquad (17)$$

where

```
Eij (ilon,ilat,iz): 3-D Emission field (in kg m-2 s-1) of a given
  species for source sector i within a grid cell with ilon, ilat
  and iz indices for latitude, longitude and vertical coordinate,
  respectively
n: total number of source sectors, which in most cases will be 1
   (e.g. it is not expected to include various 3-D emission fields
   to account for different aircraft sources of NOx)
```

All resulting diagnostics are emission rates in “kg m-2 s-1”.

Two additional routines, the module UKCA_EMDIAGS_STRUCT_MOD and the subroutine UPDATE_EMDIAGSTRUCT (also present in a module), are used by the new emission diagnostics code. UKCA_EMDIAGS_STRUCT_MOD defines the TYPE emdiags_struct, which includes for each emission diagnostic a flag indicating whether it has been previously selected from STASH (e.g. l_co for carbon monoxide emissions) as well as a pointer to hold the diagnostic values (e.g. em_co (:,:)). UPDATE_EMDIAGSTRUCT declares the derived type structure emdiags as

```
TYPE (emdiags_struct) :: emdiags
```

initialises the flags the first time it is called (e.g. emdiags%l_co=.FALSE.), and updates the fields in the structure when required. Note that the first time a diagnostic is requested the corresponding flag is set to true (e.g. emdiags%l_co=.TRUE.) and the emission values (e.g. emdiags%em_co (:,:)) are allocated. Then for simplicity the flag will remain as TRUE for the rest of the simulation while the emission values will be updated only when requested by STASH in a given time step.

UKCA_EMISS_DIAGS can generate diagnostics for each of the elements in em_chem_spec, but it does not consider online emissions such as NO_x from lightning or CH_4 from wetlands. Their corresponding diagnostics are stored in emissions(:)%diags (:,:,:) but they are not used here because their values of emissions(:)%tracer_name are respectively ‘NO_lightng’ and ‘CH4_wetlnd’, which do not match any field in em_chem_spec. Diagnostics for these two online emission fields can be output in other parts of the code: ASAD_3D_EMISSIONS_DIAGNOSTICS (called from UKCA_NEW_EMISS_CTL) for lightning emission diagnostics (section 50, items 081-086) and UKCA_MAIN1 for the CH_4 wetland emission diagnostic (section 8, item 242).

11.3 Top-level emission routine, UKCA_NEW_EMISS_CTL

This is the detailed flow of the code within UKCA_NEW_EMISS_CTL:

- In the first time step the subroutine UKCA_EMISS_INIT (contained in module UKCA_EMISS_MOD) is called to identify all NetCDF emission files, look for the emission fields present in them as well as those calculated online within UKCA, and then allocate all variables in the emissions structure.
- In the first time step the subroutine VERTIC_EMISS_FACTORS is called to get information on how to spread emissions over different vertical levels and create vertical scaling factors which are stored as 3-D arrays in the emissions structure: emissions(:) %vert_scaling_3d (1:row_length, 1:rows, 1:model_levels).
- At each time step the subroutine UKCA_EMISS_UPDATE (contained in the module UKCA_EMISS_MOD) is called to identify whether it is necessary to read each of the NetCDF emission fields for that given time. That will be done not more often than every full hour, depending on the update frequency present as a global attribute in each of the NetCDF files. When a field needs to be updated then UKCA_EMISS_UPDATE reads the emission values from the NetCDF file and stores them in the emissions structure as emissions(:) %values(:,:,:). The corresponding value of emissions(:)%l_update is also set to TRUE in that subroutine to indicate that the field has been updated at that time step.
- Call UKCA_LIGHT_CTL to get lightning emission of NO_x.
- Loop through all emission fields (both those read from NetCDF files and those calculated online) and do as follows:
  - Check emissions(:)%l_update to identify if the field has been updated in that time step. If so then call BASE_EMISS_FACTORS to get the appropriate factor and convert emission(:)%values to the right units (i.e. kg of the emitted tracer per m^2 per s) if needed. Some additional corrections are done if the field is reported in kg per grid cell. That should never be the case for emission fields present in NetCDF files (as shown in Section 11.4, CF conventions only allow units = "kg m-2 s-1"), but it might still be possible for online emission fields as it is the case for NO_x emissions from lightning.
  - If the emission field corresponds to biogenic isoprene then the subroutine UKCA_DIURNAL_ISOP_EMS is called to apply a diurnal cycle to the most recently updated emission value, which is stored in the array biogenic_isop (:,:). Note that the following variables in the emissions structure have to be as follows for biogenic isoprene emissions:

    ```
    emissions(:)%tracer_name = 'C5H8'
    emissions(:)%hourly_fact = 'diurnal_isopems'
    ```

    These two variables have been read from the attributes tracer_name and hourly_scaling of the field in the NetCDF file (see Section 11.4, in particular Table 21).
- Call the subroutine UKCA_ADD_EMISS to inject emissions and do tracer mixing. Note that the variables emission(:)%values already include units conversions. Because of that UKCA_ADD_EMISS only applies hourly, daily and vertical scaling if needed.

- Call the subroutine UKCA_EMISS_DIAGS to output emission diagnostics if any of those diagnostics has been selected via STASH.

Table 19: Description of the derived type variables contained in the emissions data structure of the new UKCA emission code.

Field in emissions structure	Description	Notes
emissions(:)%file_name	Name of source emission file	Empty if emission calculated online
emissions(:)%var_name	Name of variable in emission file	Used mainly for debugging purposes
emissions(:)%tracer_name	Emitted species	Should match one of the values in array em_chem_spec of the chemistry scheme
emissions(:)%std_name	'standard_name' attribute read from NetCDF files	Names separated by underscores (empty if there is no appropriate name that complies with CF conventions)
emissions(:)%lng_name	'long_name' attribute read from NetCDF files	Names separated by white spaces
emissions(:)%units	Units of the emission field	Always 'kg m-2 s-1' if read from a NetCDF file
emissions(:)%update_freq	Update frequency (hours)	Integer, highest frequency allowed is 1 h
emissions(:)%update_type	1 for time series 2 for periodic emissions	0 for 'single time' may be introduced in the future
emissions(:)%l_update	TRUE if emission field updated in a given timestep	In general, TRUE when model time since start is multiple of update_freq. Always TRUE for online emissions. Some operations are allowed in UKCA_NEW_EMISS_CTL only when this field is TRUE
emissions(:)%three_dim	Logical, TRUE if 3-D emission field	
emissions(:)%base_fact	Base conversion factor (used to convert units)	Equal to 1.0 if no unit conversion needed
emissions(:)%hourly_fact	Character variable indicating type of hourly scaling factor	See possible values in subroutine HOURLY_EMISS_FACTORS (in module UKCA_EMISS_FACTORS)

Table 19: Description of variables in emissions data structure – Continued

Field in emissions structure	Description	Notes
emissions(:)%daily_fact	Character variable indicating type of daily scaling factor	See possible values in subroutine DAILY_EMISS_FACTORS (module UKCA_EMISS_FACTORS)
emissions(:)%vert_fact	Character variable indicating type of vertical scaling factor	See possible values in subroutine VERTICAL_EMISS_FACTORS (in UKCA_EMISS_FACTORS)
emissions(:)%vert_scaling_3d (:,:,:)	3-D array holding vertical scaling factors for all model grid cells	Same size as model grid. It is filled in according to the value of the string emissions(:)%vert_fact
emissions(:)%lowest_lev	Lowest level where high/single level emissions can be injected	Integer value between 1 and model_levels
emissions(:)%highest_lev	Highest level where high/single level emissions can be injected	Integer value between 1 and model_levels
emissions(:)%values (:,:,:)	3-D array holding the emission values	nr of elements of third dimension is 1 for 2-D emissions and model_levels for 3-D emissions
emissions(:)%diags (:,:,:)	3-D array holding emission diagnostics	Same dimensions as emissions(:)%values (:,:,:)

11.4 Requirements for the NetCDF emission datasets

The NetCDF files with emission data may contain only one or several emission fields each one. The file names are input to the UM through the UKCA_RUN namelist and the code identifies the emission fields included in them. The only limitation is on the maximum number of files, which should not exceed 40. There is no limitation about the number of emission fields or about how to distribute them among different files. However, if many fields representing different source sectors are present it might be convenient to group those corresponding to the same emitted tracer within one single NetCDF file, as done to test this code; another option might be to group them by source sector.

All the NetCDF emission files created to test this new code comply with CF-1.5 and Met Office NetCDF conventions:

- Information on CF conventions: `http://cf-pcmdi.llnl.gov/documents/cf-conventions`
- Information on the Met Office NetCDF (MO-NetCDF) Metadata Specification: `http://fcm9/projects/FormatGovernance/wiki/MO-NetCDFDocs`. In particular see the pdf version from November 2012 available on that page.

The script cfchecker (available on Linux) is used to check that the files are CF-compliant.

All emission files have the following dimensions: longitude, latitude, vertical coordinate (scalar for 2-D emissions and vector for 3-D emissions) and time (unlimited dimension).

Each emission field in the NetCDF files needs to include the following metadata attributes so that it can be appropriately handled by the new emission code of UKCA:

- name: Name of the emission field. It does not need to follow any specific conventions but has a maximum length of 80 characters. It is a short name that is mainly used for debugging purposes within the UKCA code.
- standard_name: It should be included if an appropriate name is present in the CF Standard Name Table (see `http://cf-pcmdi.llnl.gov/documents/cf-standard-names`). At present time, the most recent version of the table is `http://cf-pcmdi.llnl.gov/documents/cf-standard-names/standard-name-table/23/cf-standard-name-table.html`. An example of a valid 'standard_name' is: "tendency_of_atmosphere_mass_content_of_nitrogen_monoxide_due_to_emission" (note that all substrings have to be separated by underscores).
- long_name: It is recommendable but only compulsory if there is no 'standard_name' available for that emission field. There are no specific CF conventions for standard names, but within the UKCA code all substrings should be separated by white space as shown in this example: "tendency of atmosphere mass content of nitrogen monoxide due to emission". The reason for this is given in the description of the attribute units.
- tracer_name: This attribute has to be equal to the name of a tracer (or of an emission field such as 'NO_aircrft') present in the list of emissions for the given chemical scheme, i.e. em_chem_spec. This name is used by the subroutine UKCA_ADD_EMISS to add the emission field to the corresponding tracer. There should be at least one emission field with the value of tracer_name equal to one of the items in em_chem_spec, otherwise the subroutine UKCA_EMISS_INIT (in module UKCA_EMISS_MOD) will report a missing tracer in the emission files and the model will stop with error.
- units: According to CF conventions, all emissions should be expressed in kg m-2 s-1. As a consequence, all files will contain the attribute

  ```
  units = "kg m-2 s-1"
  ```

  However, under some circumstances emission fields need to be reported as kg of a given species (e.g. nitrogen, carbon, sulfur). When that is the case this needs to be indicated in the standard_name attribute if possible (see example below), otherwise in the long_name attribute. As an example, in the case of an emission field reported as kg of carbon, the attribute units will be "kg m-2 s-1" while the attribute standard_name should contain the substring "expressed_as_carbon" if that is accepted by CF conventions for standard names (see `http://cf-pcmdi.llnl.gov/documents/cf-standard-names`); otherwise the attribute long_name should contain the substring "expressed as carbon". The UM subroutines BASE_EMISS_FACTORS and GET_BASE_SCALING will look for such substrings and apply some conversions if needed. It is therefore essential that the substrings in standard_name and long_name are separated by underscores and white spaces, respectively, as indicated above.

- hourly_scaling, daily_scaling and vertical_scaling: These attributes are read as characters from UKCA_EMISS_MOD and then passed to the subroutines in the module UKCA_EMISS_FACTORS, which get the corresponding numeric scaling factors to apply temporal or vertical profiles to the emission fields. When introducing some temporal or vertical scaling factors as attributes in the NetCDF files, the user will need to check whether they are considered in UKCA_EMISS_FACTORS and otherwise adapt the code in that module. In the case of climate jobs with a 360-day calendar, no weekly cycle of emissions is expected and therefore the attribute daily_scaling which indicates day-to-day variability in emissions needs to be empty or equal to 'none'. When an isoprene emission field (with attribute tracer name = 'C5H8') is expected to follow a diurnal cycle as calculated by the UM subroutine UKCA_DIURNAL_ISOP_EMS then the attribute hourly_scaling should be exactly equal to 'diurnal_isopems'. Moreover, there are two additional attributes (lowest_level and highest_level) that need to be present to indicate the lowest and highest model layers (integers) at which an emission field can be injected if the vertical_scaling is 'high_level' or 'single_level'.

In addition, each NetCDF file has to include two global attributes with information that is valid for all emission fields present in the file:

- update_freq_in_hours: Integer number indicating the frequency (in hours) at which all emission fields present in that file should be read to update emissions(:)%values (:,:,:) in the UKCA code
- emission_type: Integer number indicating the times at which the data is provided. The same conventions as for ancillary files have been adopted:

  ```
  0: Single time (not allowed yet)
  1: Time series
  2: Periodic time series
  ```

  When emissions are treated as time series (emission_type=1) the user is responsible for creating emission fields which cover the whole period for which the model is run; otherwise the model will not find the time registers to do interpolations and will stop with error. When emissions are periodic (emission_type=2) each emission field has to include exactly 12 monthly average emissions (Jan, Feb, ..., Dec).

All the mentioned attributes will be read by the UKCA code and stored in the emissions structure as indicated in Table 21. Note that the UKCA code also calculates some emission fields online and fills in the corresponding variables in the emission structure even when they have not been read from NetCDF attributes.

Other attributes, in particular some global attributes, as well as some additional fields (e.g. a variable indicating the type of grid mapping) should be present in the files to comply with CF and Met Office conventions for NetCDF data, but they are not used by the UKCA code. Section 11.4.1 provides an example of one of the NetCDF emission files used to test this code with the RAQ chemistry scheme. Some TIDL routines to generate appropriate NetCDF files for the RAQ scheme are available at: `http://fcm9/projects/utils/browser/AQ_Emissions/branches/dev/`

`cordonez/netcdf_emissions/Processing_code/Graphics_code/cdf`. At present time the code is run from

`els022:/data/local/cordonez/AQ_Emissions/code/netcdf_emissions`

These routines convert emission fields already available in pp format to NetCDF, and then add the required metadata attributes.

11.4.1 Sample of a NetCDF emission file

This section illustrates an example of a NetCDF emission file used to test the new emission code with the RAQ chemistry scheme. It includes various fields to account for several sources of nitrogen monoxide (NO) and has been tested in an AQUM (Air Quality in the Unified Model) configuration at around 12 km horizontal resolution over the UK and surrounding countries. File available on:

`hpc2e:/data/cr/atdisp/cordonez/AQ_Emissions/2010/netcdf/`
`vertfact_emep_modif_timefact_traffic_1hfreq_cyclic/aqum_srf_2010_NO.nc`

The following lines show the result of running “ncdump -c” on that file (note that the command ncdump is available on Linux but not on the HPC):

```
netcdf aqum_srf_2010_NO {
dimensions:
        longitude = 146 ;
        latitude = 182 ;
        hybrid_ht = 1 ;
        time = UNLIMITED ; // (12 currently)
variables:
        float longitude(longitude) ;
                longitude:units = "degrees" ;
                longitude:point_spacing = "even" ;
                longitude:standard_name = "grid_longitude" ;
                longitude:long_name = "longitude in rotated pole grid" ;
        float latitude(latitude) ;
                latitude:units = "degrees" ;
                latitude:point_spacing = "even" ;
                latitude:standard_name = "grid_latitude" ;
                latitude:long_name = "latitude in rotated pole grid" ;
        float hybrid_ht(hybrid_ht) ;
                hybrid_ht:units = "metre" ;
                hybrid_ht:positive = "up" ;
                hybrid_ht:standard_name = "height" ;
                hybrid_ht:long_name = "height at theta layer midpoint" ;
        float time(time) ;
                time:units = "days since 2010-01-01 00:00:00" ;
                time:time_origin = "01-JAN-2010:00:00:00" ;
```

```
                time:standard_name = "time" ;
                time:long_name = "time" ;
                time:calendar = "gregorian" ;
        char rotated_pole ;
                rotated_pole:grid_mapping_name = "rotated_latitude_longitude" ;
                rotated_pole:grid_north_pole_longitude = 177.5f ;
                rotated_pole:grid_north_pole_latitude = 37.5f ;
                rotated_pole:earth_radius = 6371229.f ;
        float NO_emissions_snap01(time, hybrid_ht, latitude, longitude) ;
                NO_emissions_snap01:name = "NO" ;
                NO_emissions_snap01:long_name = "tendency of atmosphere mass
content of nitrogen monoxide due to emission from SNAP sector 01" ;
                NO_emissions_snap01:units = "kg m-2 s-1" ;
                NO_emissions_snap01:missing_value = 2.e+20f ;
                NO_emissions_snap01:_FillValue = 2.e+20f ;
                NO_emissions_snap01:valid_min = 5.74510781968533e-21 ;
                NO_emissions_snap01:valid_max = 7.03106572963463e-10 ;
                NO_emissions_snap01:standard_name =
 "tendency_of_atmosphere_mass_content_of_nitrogen_monoxide_due_to_emission" ;
                NO_emissions_snap01:tracer_name = "NO" ;
                NO_emissions_snap01:emiss_sector = "snap01" ;
                NO_emissions_snap01:hourly_scaling = "traffic_uk" ;
                NO_emissions_snap01:daily_scaling = "traffic_uk" ;
                NO_emissions_snap01:vertical_scaling = "EMEP_modified_SNAP01" ;
                NO_emissions_snap01:grid_mapping = "rotated_pole" ;
........

        float NO_emissions_snap10(time, hybrid_ht, latitude, longitude) ;
                NO_emissions_snap10:name = "NO" ;
                NO_emissions_snap10:long_name = "tendency of atmosphere mass
 content of nitrogen monoxide due to emission from SNAP sector 10" ;
                NO_emissions_snap10:units = "kg m-2 s-1" ;
                NO_emissions_snap10:missing_value = 2.e+20f ;
                NO_emissions_snap10:_FillValue = 2.e+20f ;
                NO_emissions_snap10:valid_min = 6.28819278637572e-22 ;
                NO_emissions_snap10:valid_max = 7.69571212311249e-11 ;
                NO_emissions_snap10:standard_name =
"tendency_of_atmosphere_mass_content_of_nitrogen_monoxide_due_to_emission" ;
                NO_emissions_snap10:tracer_name = "NO" ;
                NO_emissions_snap10:emiss_sector = "snap10" ;
                NO_emissions_snap10:hourly_scaling = "traffic_uk" ;
                NO_emissions_snap10:daily_scaling = "traffic_uk" ;
                NO_emissions_snap10:vertical_scaling = "EMEP_modified_SNAP10" ;
```

```
                NO_emissions_snap10:grid_mapping = "rotated_pole" ;

// global attributes:
                :history = "Thu May 9 17:33:05 2013: Created by routine
           els022:/data/local/cordonez/AQ_Emissions/code/netcdf_emissions/
           Processing_code/Graphics_code/cdf/pp_copy2_nc_snap.pro" ;
                :update_freq_in_hours = "1" ;
                :emission_type = "2" ;
                :Conventions = "CF-1.5, UKMO-1.0" ;
                :title = "UKCA-RAQ emissions" ;
                :institution = "UK Met Office" ;
                :source = "NAEI + EMEP + ENTEC emission inventories" ;
                :IDL = "8.2" ;
}
```

12 Top boundary conditions

As the tropospheric chemistry schemes do not include chemical reactions essential to model the production and loss of ozone in the stratosphere, a method has to be used to correctly parameterise the O_3, CH_4, and reactive N species at the top boundary of the model using a source of data external to the chemistry scheme being used. Various options control the functioning of this code which is in routine UKCA_STRATF. The following describes the default settings in this routine.

12.1 Stratospheric methane loss

For methane, the model calls a subroutine ukca_ch4_stratloss in which an explicit loss rate is applied to CH_4 in the top 3 levels of the model. This routine is only called by the chemical schemes using the Backward-Euler solver. The loss rate used (2.0×10^{-7}) should give a stratospheric loss of approximately 40 Tg (CH_4)/year in present-day simulations, in line with Prather et al. (2001). In the UKCA_STRATF code, the logical L_overwrite_CH4 is set to false, so methane is not overwritten here using data from the Cambridge 2D model (Law and Pyle (1993)). For long runs the value of the loss rate should be tuned to give an acceptable value.

12.2 Specifying the ozone concentration

The UM ozone ancillary data is used as the top boundary condition and is the default option in the code as the logical L_USE_UMO3 = .true. It uses the same ozone field (e.g. SPARC or Rosenlof climatology) that is used to drive the UM radiation scheme (Edwards and Slingo (1996)) which may evolve with time. In this case, O_3 is overwritten on model levels which are equal or above to a fixed number of levels above the diagnosed tropopause. The number of levels used will depend on the number of vertical levels in the model.

When the logical L_USE_UMO3 = .false. then ozone data from the Cambridge 2D model (Law and Pyle (1993)) is used.

12.3 Specifying the NO_y concentration

The selection of the NO_y data source is specified by the logical L_use_O3HNO3_ratio which is by default set to true in the code. The default approach is to use a fixed O_3:HNO_3 ratio from (Murphy and Fahey (1994)) and is used to simply overwrite HNO_3. All other NO_y species are not overwritten. If L_use_O3HNO3_ratio is changed to false, the Cambridge 2D model data are used to specify NO, NO_3, NO_2, N_2O_5, HNO_3, and HO_2NO_2.

12.4 Specifying the overwriting behaviour

The default behaviour in UKCA_STRATF (L_use_O3HNO3ratio and L_all_strat are both set to true) is to overwrite the stratospheric concentrations at least 3 levels above the diagnosed tropopause. Where the logicals are set differently, the stratospheric concentrations are overwritten where the pressure is below 7000 Pa.

12.5 Input from the Cambridge 2D model

The Cambridge 2D data (Law and Pyle (1993)) is not used as a default because the output from the 2D model is only for a single year and is not appropriate for a long transient model integration. For methane, the 2D approach is too strong a sink for CH_4 in the present day and acts as a source of CH_4 in the preindustrial period.

13 GLOMAP-mode: the UKCA Aerosol Scheme

13.1 Overview of GLOMAP-mode

13.1.1 Introduction

The Global Model of Aerosol Processes (GLOMAP) simulates the evolution of size-resolved aerosol properties, including processes such as new particle formation, coagulation, condensation (gas-to-particle-transfer) and cloud processing. Prognostic variables in GLOMAP are particle number and mass concentrations in different size classes (from $\approx 3\,\mathrm{nm}$ up to $\approx 25\,\mu\mathrm{m}$ dry diameter). Processes such as condensation and aqueous sulphate production grow particles by increasing the mass in a size class while conserving particle number. The model includes size-resolved representations of primary emissions (e.g. sea-salt, dust and carbonaceous particles) and of several removal processes including particle dry deposition, sedimentation, nucleation scavenging (rainout) and impaction scavenging (washout).

GLOMAP simulates the evolution of particle composition across the size spectrum over several different components as determined by the aerosol processes included. The original version of GLOMAP (known as GLOMAP-bin) uses a two-moment sectional aerosol dynamics approach (e.g. Spracklen et al. (2005)), with typically 20 bins spanning the size spectrum, but when tracking several aerosol types, becomes too expensive for running multi-decadal integrations as required in a climate model. For UKCA, a new computationally cheaper version of GLOMAP was developed (GLOMAP-mode), which has the same process representations, but using log-normal modes as its size classes. Each size mode in GLOMAP-mode covers one of four size ranges, with additional separation among soluble and insoluble modes (see Table 22), following the framework of the M7/HAM aerosol microphysics scheme (Vignati et al. (2004); Stier et al. (2005)). GLOMAP has been developed to follow a flexible multi-component approach, with the same code able to be run with different levels of composition/size sophistication with Fortran modules providing alterative aerosol "mode set-up" arrays.

13.1.2 Aerosol processes and the mapping to size modes

New particle formation generates sub-10nm sulphate particles within a nucleation mode, and primary-sulphate (sub-grid-scale particle formation) can emit into larger Aitken and accumulation modes. Carbonaceous aerosol emits into an insoluble Aitken mode and dust emits into insoluble accumulation and coarse modes and are transferred to their corresponding soluble mode following the "condensation-ageing" approach described in Wilson et al. (2001). Sea-salt is emitted into soluble accumulation and coarse soluble modes where it can become internally mixed with sulphate and aged BC/OC and dust. The GLOMAP-mode code calculates sources and sinks (and inter-modal transfer) of number and mass for each of these modes and a mode-merging where particles grow outside prescribed mode edge radii.

13.1.3 Host model implementation and recent improvements

GLOMAP was originally developed as an extension to the 3D global offline chemistry transport model TOMCAT (Chipperfield (2006)). The aerosol processes solved in an operator-split manner, with the gas phase chemistry and transport dealt with separately, within the host model, which can be a CTM or a general circulation model.

Mann et al. (2010) comprehensively describe GLOMAP-mode and its implementation within TOMCAT (driven by offline oxidant fields from a previous full chemistry run), showing evaluation of simulated aerosol properties against a range of global observational datasets. Several science papers have used this “offline-oxidant” TOMCAT implementation of GLOMAP-mode (e.g. Manktelow et al. (2007); Woodhouse et al. (2011); Spracklen et al. (2011); Lee et al. (2011); Browse et al. (2012)) and an alternative TOMCAT configuration of GLOMAP-mode, where the aerosol precursor gases are fully coupled to the TOMCAT tropospheric chemistry scheme, has also been developed (e.g. Breider et al. (2010); Schmidt et al. (2010); Schmidt et al. (2011)).

Recently, GLOMAP-mode has also been improved (Mann et al. (2012)) by comparing simulated size distributions in the CTM environment against those from the sectional GLOMAP-bin scheme (Spracklen et al. (2005); Merikanto et al. (2009)) in the same model. During this benchmarking, several improvements to the GLOMAP-mode aerosol scheme have been made, including changes to the process formulations for vapour condensation (condensation-diameter used as representative size of the mode) and nucleation scavenging (uses size-threshold to determine scavenging coefficients for each mode) to better match approaches in GLOMAP-bin. These improvements are described in Mann et al. (2012). As well as the process formulation changes, the prescribed geometric standard deviation has been narrowed from 1.59 to 1.40 in the accumulation-soluble mode to better compare against GLOMAP-bin (see Table 22). Also, the mode-edge radius separating accumulation and coarse soluble modes has been reduced from 500nm to 250nm to minimise problems where ultra-fine sea-spray particles are mixed with cloud-processed Aitken mode particles in the accumulation mode.

13.2 GLOMAP-mode aerosol configurations

The main GLOMAP-mode configuration (mode setup 2, MS2) used in MetUM (as described in Johnson et al. (2010)) is to have dust treated by the existing MetUM 6-bin dust scheme (Woodward (2001)) with GLOMAP-mode simulating sulphate, BC, OC and sea-salt in 5 modes (20 aerosol tracers).

However, as described above, GLOMAP-mode can be run with several possible aerosol configurations (referred to as “mode set-ups”, see Tables 23 and 24). For instance, in TOMCAT-GLOMAPmode, the standard GLOMAP-mode configuration (as described in Mann et al. (2012)) has dust included within the UKCA modal framework, with all 7 modes active (MS8). Another possible GLOMAP-mode set-up (MS4) neglects dust but allows secondary organic aerosol mass to be tracked separately from primary organic carbon mass in a second OC component (OC2) in the 4 soluble modes as used in TOMCAT-GLOMAPmode by Spracklen et al. (2011).

A simpler configuration (MS1) neglects both dust and carbonaceous aerosol components, tracking only sulphate and sea-salt mass components in just 4 soluble modes. This configuration was used in HadGEM3-UKCA to study changes to stratospheric aerosol after the Pinatubo eruption (Emmerson et al. (2012, in prep.)). Note however, that although these stratospheric aerosol simulations have been carried out extensively at MetUM version v7.3, and the necessary code updates lodged to the MetUM trunk at v8.2, that part of the code is untested at present.

13.3 Implementation of GLOMAP-mode within UKCA

13.3.1 Overview of GLOMAP-mode

The GLOMAP-mode routines are all called off one master routine UKCA_AERO_STEP in a sequential, process-split fashion. Each of the GLOMAP-mode routines operates by updating the two key arrays “ND” and “MD” which (respectively) store the particle number concentration in each mode (per cubic centimetre), and the mass (in molecules per particle) of each of the aerosol components (sulphate, sea-salt, BC, POM, dust, etc.) in each mode. The array S0G stores the masses of the gas phase tracers and those gas phase tracers that are condensible are also stored in a local array GC.

The GLOMAP-mode processes apply equations to update GC/S0G, ND and MD across the modes according to the process involved. For instance, a growth process (such as in-cloud sulphate production or condensation of sulphuric acid into the aerosol phase) will increase the MD value for sulphate in a particular mode, but will not change that mode's ND value. A process removing mass from the gas phase (such as condensation of sulphuric acid or nucleation) will additionally decrease GC/S0G to account for the sink of that gas.

The interface routine for calling the GLOMAP-mode routines within UKCA is UKCA_AERO_CTL, which itself is called from UKCA_MAIN after UKCA_CHEMISTRY_CTL. UKCA_AERO_CTL essentially sets up all the input switches/variables/arrays required by UKCA_AERO_STEP, mapping from arrays in the UM or UKCA.

An important part of UKCA_AERO_STEP is where the key GLOMAP-mode aerosol arrays ND and MD are set, so this is described briefly here. The advected GLOMAP-mode aerosol tracers (see Table 23) are all treated as mixing ratios in the UM advection routines, with the number-in-each-mode stored as a "number-mixing-ratio", i.e. the ratio of the particle number concentration to the molecular concentration of air. These GLOMAP-mode aerosol tracer mixing ratios are passed into UKCA_AERO_CTL via the mode_tracers array. Within UKCA_AERO_CTL, each of the entries in mode_tracers are then mapped onto the ND and MD arrays to be operated on under UKCA_AERO_STEP. Index arrays II_ND(NMODES) and II_MD(NMODES,NCP) are used to map between the mode_tracers and MD/ND. The ND values for mode IMODE (in particles per cubic centimetre) are derived from the II_ND(IMODE) entry in mode_tracers with multiplication by the molecular air density (AIRD). The MD values are derived from the II_MD(IMODE,ICP) entry in mode_tracers with multiplication by AIRD, dividing by the ND value for the mode, and multiplying by the ratio of the molar mass of dry air (MM_DA) to that of the aerosol component (MM(ICP)). The latter scaling is required because the mode-aerosol-masses in mode_tracers are mass mixing ratios (for instance kg of sodium chloride per kg of air for sea-salt mass) whereas the MD values are in molecules per particle, so MD times ND divided by AIRD is effectively a volume mixing ratio.

13.3.2 Inputs/outputs to/from GLOMAP-mode from UKCA chemistry

As described in Mann et al. (2010), the GLOMAP-mode code includes a routine "UKCA_WETOX" to calculate the in-cloud-droplet aqueous sulphate production via reaction of dissolved SO2 with dissolved H_2O_2 and O_3. When GLOMAP-mode is run in the TOMCAT chemistry transport model, the ASAD chemistry module is used, but that only covers the gas phase reactions for the aerosol chemistry. For the aqueous phase sulphate production, the GLOMAP-mode routine UKCA_WETOX is used, which calculates the rate of conversion of SO_2 into aerosol sulphate mass (using input concentrations of SO_2, H_2O_2 and O_3) and also has a scheme to calculate the replenishment of H_2O_2 via gas-phase self-reaction of HO_2 up to a maximum background concentration $H_2O_{2,max}$. However, when the GLOMAP-mode code is run within UKCA, the aqueous reactions are included within the UKCA chemistry module as part of the "aerosol-chemistry" (see section 5) added to the standard UKCA chemistry schemes as summarized in Table 2.

To allow the same GLOMAP-mode routines to be used in both TOMCAT and MetUM, there is a switch “WETOX_IN_AER” to determine whether the aqueous chemistry is to be done in the GLOMAP-mode aerosol schemes or not. When GLOMAP-mode is run in TOMCAT, the routine UKCA_WETOX needs to be set to 1, and the concentrations of SO_2, H_2O_2 are passed in to UKCA_AERO_STEP via the S0/S0G input array, whereas O_3 HO_2, and $H_2O_{2,max}$ are passed in via the input arrays ZO3, ZHO2 and ZH2O2. The outputs from UKCA_WETOX to UKCA_AERO_STEP are the arrays DELSO2 and DELSO2_2 which contain the conversion rates for gas phase SO_2 to aerosol sulphate via the aqueous reactions with H_2O_2 and O_3 respectively. When GLOMAP-mode is run in MetUM however, the switch WETOX_IN_AER is set to zero and the code then expects the arrays DELSO2 and DELSO2_2 to be provided as input. With this approach, DELSO2 and DELSO2_2 are set in UKCA_AERO_CTL are set from arrays delso2_wet_h2o2 and delso2_wet_o3 which store the aqueous sulphate production rate as calculated under UKCA_CHEMISTRY_CTL.

Under UKCA_AERO_STEP, in the routine UKCA_CONDEN, the GLOMAP-mode code calculates the condensation of gas phase sulphuric acid and the condensible organic species ”SEC_ORG” (see Table 10). Another key part of UKCA_AERO_CTL, which requires some explanation, is that the tendencies and concentations of these two condensible gas phase species are calculated along with the rest of the gas phase species under UKCA_CHEMISTRY_CTL, but the condensible species are only updated on the short “microphysics-timestep” (there are NZTS of these, usually 5). To allow this to happen, the net production/destruction (tendency) for these condensible species is pass in as input to UKCA_AERO_STEP via the array S0G_DOT_CONDENSABLE, so that the chemical tendency can be applied to update the condensible tracer concentrations on the same short microphysics timestep as they are updated for the sinks due to nucleation of new aerosol particles and condensation onto existing particles. Again, there is a switch “uph2so4inaer” (renamed to “DRY_OX_INAER” in UKCA_AERO_CTL and UKCA_AERO_STEP) which allows this approach to be switched on or off. If uph2so4inaer is set to 1, then in UKCA_CHEMISTRY_CTL, after the chemistry has been integrated, the H_2SO_4 tracer entry in the main tracer arrays (“y” for the Newton-Raphson options) are re-set to the value before the chemistry was integrated (via the array ”ystore” for the Newton-Raphson options) and the array “delh2so4_chem” is set according to the net chemical production from the termolecular SO_2 reaction with OH and the destruction via photolysis (if included). The delh2so4_chem array is then passed out of UKCA_CHEMISTRY_CTL and passed in to UKCA_AERO_CTL where it is copied to the S0G_DOT_CONDENSABLE array and passed in to UKCA_AERO_STEP to allow the H_2SO_4 entry in S0/GC to be updated on the short timestep consistently with the updating due to condensation and nucleation.

The input arrays required by UKCA_AERO_STEP to allow the gas phase species to be updated and returned are thus S0 and S0_DOT_CONDENSABLE. In UKCA_AERO_CTL, there is code to set the required entries to S0 from the entries in the array “chemistry_tracers”, which stores the full array of the UKCA gas phase tracers. If WETOX_IN_AER and uph2so4inaer / DRYOX_IN_AER are set to 0 and 1 respectively (the usual settings for use within UKCA), then only the S0 entry for SEC_ORG is required to be set, with the S0G_DOT_CONDENSABLE entry for H_2SO_4 also set to allow the sulphuric acid tracer in S0/GC to be updated under UKCA_AERO_STEP. Additionally, the DELSO2 and DELSO2_2 are set from the arrays delso2_wet_h2o2 and delso2_wet_o3 passed in from UKCA_CHEMISTRY_CTL.

Outputs from the GLOMAP-mode aerosol scheme used by the UKCA chemistry are surface area density and each mode’s geometric mean radius which can be used for the tropospheric heterogeneous chemistry described in section 4.6. Also, the aerosol surface area density simulated by GLOMAP-mode can be used in the calculated heterogeneous reaction rates in the UKCA stratospheric chemistry scheme

(Table 2). Note however that, although this latter option has been tested for heterogeneous conversion of N_2O_5 to HNO_3 in the vn7.3 UKCA Pinatubo study, it has not been tested at vn8.2.

13.3.3 The GLOMAP-mode modules

There are two FORTRAN-90 modules within the GLOMAP-mode code which allow the same GLOMAP-mode subroutines to be run with the various aerosol configurations listed in Table 23. The first module, UKCA_MODE_SETUP, has several alternative "module-procedures" which, for the chosen aerosol set-up (MS value), set the values for several basic aerosol configuration arrays and switches. For example, the arrays mode_choice and component_choice specify which modes and components are switched on, and the arrays MM and RHOCOMP set the molar masses and densities for each of the aerosol components. The second module is called UKCA_SETUP_INDICES, and sets the values of tracer and budget-flux indices for the various aerosol configurations supported under this version.

The only two aerosol configurations for GLOMAP-mode that can be run within UKCA currently are Mode Setup 1 (MS1) and Mode Setup 2 (MS2). Mode Setup 1 (also known via the abbreviation SUSS_4mode) has only the 4 soluble modes switched on and includes only sulphate and sea-salt as active aerosol components in those modes. Here, sulphate is included in all four soluble modes while sea-salt is included in the accumulation and coarse soluble modes (see Table 23). For Mode Setup 2, the black carbon (BC) and particulate organic matter (OC) components are additionally included in several modes with the OC component containing primary organic matter (co-emitted in an internal mixture with BC) as well as secondary organic matter generated from monoterpene oxidation (transferring from the gas phase condensible organic tracer SEC_ORG in the UKCA_CONDEN routine).

13.3.4 Overview of UKCA_AERO_STEP

The routine UKCA_AERO_STEP forms the "spine" of the GLOMAP-mode code, calling each of the routines to update ND, MD and S0G/GC in a process-split fashion. The ordering of the routines follows that for GLOMAP-bin as in the flowchart shown in Figure 1 of Spracklen et al. (2005). First are the routines which update ND and MD for primary emissions of sulphate (UKCA_PRIM_SU), carbonaceous aerosol (UKCA_PRIM_CAR) and sea-salt (UKCA_PRIM_SS). After that, are the wet removal routines for impaction scavenging (UKCA_IMPC_SCAV) and nucleation scavenging (UKCA_NUCL_SCAV), followed by the routines for aqueous sulphate production (UKCA_WETOX) and cloud processing from Aitken to accumulation mode (UKCA_CLOUDPROC). and aerosol dry deposition and sedimentation (UKCA_DDEPAER_INCL_SEDI). Those processes listed above are all integrated with the same timestep as that for the UKCA_CHEMISTRY_CTL (typically one hour for Newton Raphson solver chemistry). Once those processes have been integrated, the chemical production for the condensables (determined by S0G_DOT_CONDENSABLE), the vapour condensation (UKCA_CONDEN), nucleation (UKCA_CALCNUCRATE), coagulation (UKCA_COAGWITHNUCL) and condensation-ageing (UKCA_AGEING) are all integrated on the shorter "microphysics timestep", of which there are NZTS to every chemistry timestep. After the end of the loop over NZTS, the re-moding routine UKCA_REMODE is then called to apply mode-merging in grid-boxes where the geometric mean radius have exceeded the specified upper-edge radius for its mode. Where that has occurred, the fraction of the number and mass in particles larger than the upper-edge radius are transferred to the next mode up as described in Mann et al. (2010).

13.3.5 Primary aerosol emissions and BL mixing in GLOMAP-mode

Primary aerosol emissions are handled from routine UKCA_EMISSION_CTL from where the routine UKCA_MODE_EMS_UM is called, and which returns the em_field_mode array, a three-dimensional array holding emissions for each GLOMAP-mode tracer where appropriate. Routine UKCA_MODE_EMS_UM imports the emission arrays provided from the specified ancillary fields, and calls the routine UKCA_MODE_EMS which in turn calls routines that generate the mass and number emissions for each aerosol species in turn. UKCA_MODE_EMS_UM also returns an updated STASHwork array containing the section 38 emission flux items.

The routine UKCA_PRIM_SU provides mass and number emissions for primary sulphate emissions, which codes that the fraction PARFRAC (usually set to 0.025 matching AEROCOM recommendations in Dentener et al. (2006)), of SO_2 emissions appears as particulate sulphate on the sub-grid-scale. The primary sulphate from anthropogenic (EMANSO2), volcanic (EMVOLCONSO2, EMVOLEXPSO2) and biomass burning (EMBIOMSO2) sources of SO_2 are all included. The emissions size distribution assumed for these sources is that given in Stier et al. (2005), and is used to give the number fluxes for each source. Primary carbonaceous emissions are generated in routine UKCA_PRIM_CAR with fossil fuel and biofuel sources passed in via array EMC and biomass burning sources passed in via EMCBM. The BC and POM from these sources are co-emitted into the model Aitken insoluble mode with an internally mixed composition and size distribution from Stier et al. (2005) assumed in determining the particle number flux. The routine UKCA_PRIM_SS generates sea-salt emissions from the 10 m scalar wind field. The Gong (2003) size-resolved source function is used. Size-resolved sea-spray fluxes are evaluated on a 20 bin size grid with bin-resolved emissions fluxes fed into either the accumulation or coarse soluble modes depending on whether they are larger or smaller than the accumulation-coarse mode edge dry-radius. Dust is not currently supported by the GLOMAP-mode emissions scheme.

13.3.6 Boundary layer mixing of GLOMAP-mode aerosol tracers

Boundary layer mixing of the GLOMAP-mode aerosol tracers is handled in a similar way to the chemical tracers by the UKCA_EMISSION_CTL routine. After the primary emissions have been evaluated (see above), the MetUM routine TR_MIX is called for each tracer. An emission value (set to zero for tracers without emissions) is supplied, with the resistance factor (res_factor) set to zero so that no dry deposition occurs. This procedure means that emissions and boundary layer mixing are now done before the call to UKCA_AERO_CTL where aerosol microphysics and deposition processes are done. This results in somewhat higher distributions of emitted aerosol species such as black carbon and sea-salt than the previous procedure when TR_MIX was called from UKCA_AERO_CTL before the emissions were applied.

13.3.7 Aerosol dry deposition and sedimentation in GLOMAP-mode

The approach for dry deposition of aerosol in GLOMAP-mode within UKCA is the same as that described in section 2.2.2 of Mann et al. (2010) with a dry deposition velocity V_{d} for each aerosol mode given as the combination of a gravitational settling velocity V_{grav} and one-over the sum of the aerodynamic and surface resistances (R_{a} and R_{s})

$$V_{\mathrm{d}} = V_{\mathrm{grav}} + \frac{1}{R_{\mathrm{a}} + R_{\mathrm{s}}} \, . \tag{18}$$

Collection efficiencies for Brownian diffusion, impaction and interception are set following Zhang et al. (2001) mapping the 16 types given there onto the 9 UM land-surface categories. Note however that the current code does not use the UM sub-grid land-surface types explicitly. Instead, in UKCA_AERO_CTL, the value of the surface roughness length ZNOT is used to specify a single land-surface type for each gridbox, matching the approach used in TOMCAT-GLOMAP-mode. Gridboxes with ZNOT below 1mm are assumed to be water/sea, while those with ZNOT above 0.1m are assumed to be forest. Values in between are set to be grassland. For gridboxes with more than 50% sea-ice cover, the gridbox land-surface category is set as sea-ice.

Average particle diffusion coefficients (D_{coff}) for number and mass are computed for each mode in the routine UKCA_DCOFF_PAR_AV_K as:

$$D_{\mathrm{coff},k} = D_{\mathrm{coff}} \left\{ \exp\left(\frac{(-2k+1)}{2} \log^2 \sigma_{\mathrm{g}} \right) + 1.246 \frac{2\lambda_{\mathrm{a}}}{D_{\mathrm{p}}} \exp\left(\frac{(-4k+4)}{2} \log^2 \sigma_{\mathrm{g}} \right) \right\} \tag{19}$$

following the approach described in Binkowski & Shankar (1995), with σ_{g} the geometric standard deviation for the mode and k the index of the moment (zero for number, three for mass). The values for D_{coff} are used to determine the particle Schmidt number, which itself determines the particle collection efficiencies for Brownian diffusion, impaction and interception (see Mann et al., 2010).

Similarly, separate values of V_{grav} are also computed for the average value for particle number and mass in each mode in the routine UKCA_VGRAV_AV_K as:

$$V_{\mathrm{grav},k} = V_{\mathrm{grav}} \left\{ \exp\left(\frac{(4k+4)}{2} \log^2 \sigma_{\mathrm{g}} \right) + 1.246 \frac{2\lambda_{\mathrm{a}}}{D_{\mathrm{p}}} \exp\left(\frac{(2k+1)}{2} \log^2 \sigma_{\mathrm{g}} \right) \right\} \tag{20}$$

to give average R_{s} values for the 0th and 3rd radial-moments, and for V_{d} from equation 18.

The change in ND and MD for combined dry deposition and sedimentation is calculated in the routine UKCA_DDEPAER_INCL_SEDI, under UKCA_AERO_STEP. Sedimentation from the lowest grid level is handled based on the dry deposition velocity as in equation 18, whereas for other levels, sedimentation is applied using $V_{\mathrm{grav},k}$ following a 1st order explicit scheme, calculating fluxes of number and mass into and out of each box. Sedimentation is limited to only half a gridbox per timestep to ensure the Courant-Fredrichs-Levy condition is satisfied.

13.3.8 Aerosol scavenging in GLOMAP-mode

Both nucleation (in-cloud) scavenging (also known as rainout) and impaction (below-cloud) scavenging (also known as washout) are included within GLOMAP-mode as separate processes.

The approach for impaction scavenging (routine UKCA_IMPC_SCAV) in GLOMAP-mode within UKCA is the same as used when the scheme is run within TOMCAT, with rain rates for large-scale (DRAIN) and convective-scale (CRAIN) precipitation used to drive the scavenging rate, based on look-up tables for collision efficiency between aerosols and raindrops (see Mann et al. (2010)).

For nucleation scavenging (routine UKCA_RAINOUT), the approach broadly follows that in Mann et al. (2010) with the size threshold approach used to determine the scavenging coefficient R_{SCAV} for each mode as described in Mann et al. (2012). This threshold is set at 103 nm as dry radius. Previously, the vertical differences in the diagnosed rainfall rate were used to determine the rate of conversion of cloud water to rainwater. However in the Global Atmosphere 4.0 configuration, a prognostic rain scheme was adopted as part of the changes intended to reduce the surface drizzle rates (Walters et al. (2011)), and vertical rain differences cannot now be used. To replace the vertical rain differences, the sum of the autoconversion, in-cloud accretion, ice melt and snow melt diagnostic rates ($AUTOCONV$) was used. The ice and snow melting rates are included for now to make the code more compatible with the previous version based on vertical rainfall differences. Evaporation of rain is not included in this version. With this approach, the rate of conversion of cloud water to rain water in the large-scale scavenging β_{LS} was derived from:

$$\beta_{LS} = \frac{AUTOCONV}{CLWC}, \tag{21}$$

where $CLWC$ is the cloud water content. The change in number concentration for the mode (N) due to nucleation scavenging by large-scale rain ΔN_{lsns} is then given by:

$$\Delta N_{lsns} = N \times R_{SCAV} \times (1 - exp(-\beta_{LS} \times \Delta t), \tag{22}$$

where Δt is the timestep. Note that the rates used are mean gridbox values, so the cloud fraction is not included here. The scavenging coefficients R_{SCAV} are set to 1.0 for the soluble coarse mode, and to zero for the nucleation mode, and is set to

$$R_{SCAV} = 1.0 - Frac$$

for the soluble Aitken and accumulation modes, where $Frac$ is the fraction of number or mass which has a radius greater than a specified activation radius, currently set at a dry radius of 103 nm. Where $Frac$ is less than 10 % of the number or mass of the mode, R_{SCAV} is set to zero. For the insoluble modes, R_{SCAV} is set to zero unless the temperature is below 258 K when it is set to 1.0 . An integer variable (i_mode_nucscav) normally set to 1 in UKCA_OPTION_MOD may be set to 2 in order to use the scavenging ratios as in the ECHAM5-HAM model Stier et al. (2005). This variable affects both the rainout and plume scavenging routines.

Rainout from the convection scheme is now normally not handled by this routine, as there is now a plume scavenging scheme which removes soluble aerosol mass as part of the convective plume calculation Kipling et al. (2013). This scheme is described below, and inhibits the convective transport of too much aerosol to regions of the model where it cannot be removed by wet processes. However, if the plume scavenging scheme is turned off, convective scavenging is added to the large scale nucleation scavenging in UKCA_RAINOUT.

13.3.9 Aerosol scavenging in the convective plume

Kipling (2013) and Kipling et al. (2013) describe a scheme that removes aerosol from the convective plume. This replaces the operator splitting technique used previously which calculated the rainout after convective tracer transport had taken place. This allowed material to be transported vertically in the convection scheme to the upper part of the model where it was out of reach of the wet scavenging scheme. In the Global Atmosphere configurations GA4.0 and above, the proportion of rainfall delivered by the convection scheme is much greater than in previous versions, and the plume scavenging scheme has been found to be an essential part of the aerosol model in order to avoid simulating aerosol optical depths which are unrealistically high. Thus the logical L_UKCA_PLUME_SCAV is set to true in routine UKCA_OPTION_MOD.

As a convective parcel ascends, it cools and may lose water as condensate. If the cloud condensate exceeds a minimum value, the excess is converted to precipitation during ascent to the next level. The change in the aerosol tracer mixing ratio during in-cloud scavenging of aerosol is described by a first order loss rate:

$$\Delta n_k^p = \frac{\alpha g P_k n_{k+1}^p}{M_{k+1} l_{k+1}^p}, \tag{23}$$

where the index k denotes the level, n_k^p is the number or mass mixing ratio in a particular mode within the parcel at level k, $n_k^p + 1$ is the mixing ratio after lifting to level $k + 1$, but before scavenging has taken place, α is the scavenging ratio, P_k is the rate at which precipitation is produced by lifting from level k to level k+1, g the acceleration due to gravity, M_k is the updraught mass flux at level k, and l_{k+1}^p is the mass mixing ratio of liquid water or ice before removal by precipitation. The factor g converts M_k from units of $Pa\ s^{-1}$ to $kg\ m^{-2} s^{-1}$, the same units as P_k. The scavenging ratio is set to 1.0 for accumulation and coarse soluble modes and to a variable fraction which is set at run time (mode_aitsol_cvscav) for the Aitken soluble mode. The fraction used in developing this module was 0.5, but further work is needed to tune this parameter. For other modes (insoluble modes and nucleation soluble), it is set to zero. An integer variable (i_mode_nucscav) normally set to 1 in UKCA_OPTION_MOD may be used to access the scavenging ratios used in the ECHAM5-HAM model Stier et al. (2005) (i_mode_nucscav=2).

liquid and ice cloud are not differentiated in the parameterisation, and Kipling (2013) states that this is effectively assuming that most of the ice particles which form in the upper part of the convective cloud originate from the freezing of liquid drops which will have taken up aerosol when they were formed.

Testing of the plume scavenging scheme has been done with the 5A convection code, it is not available for the 6A convection scheme yet. As the logical l_UKCA_PLUME_SCAV is set to TRUE in the UKCA code, if the 6A scheme is selected, plume scavenging will be turned off and a warning message written.

13.3.10 Modifications to GLOMAP-mode for the stratosphere

As explained in section 5.3, the aerosol chemistry for the UKCA stratospheric chemistry scheme consists of a sulphur chemistry scheme suitable for the stratosphere including photolytic and thermal reactions for COS, SO_2, SO_3 and H_2SO_4.

As well as adding the stratospheric aerosol chemistry, some changes to the UKCA-MODE routines were required to enable the code to be applicable to both tropospheric and stratospheric conditions. In the troposphere, sulphuric acid in the aerosol phase has essentially zero vapour pressure. In the stratosphere however, the aerosol H_2SO_4 vapour pressure becomes sigificant and in some regions of the stratosphere, evaporation of H_2SO_4 can occur and can play an important role in determining the distribution of stratospheric aerosol (Weisenstein and Bekki, 2006).

The UKCA-MODE aerosol routine for condensation UKCA_CONDEN has been modified and now calls a new routine UKCA_VAPOUR to calculate the H_2SO_4 vapour pressure allowing evaporation or condensation of sulphuric acid depending on the atmospheric conditions (following Ayers et al. (1980), as modified by Kulmala and Laaksonen (1990)). The Kelvin effect is also included in the vapour pressure calculation using the mean radius calculated by GLOMAP-mode. Note however, that, due to technical issues, at present the H_2SO_4 vapour pressure calculated in UKCA_VAPOUR is not yet used in the model, and the UKCA_CONDEN routine continues to apply a zero H_2SO_4 vapour pressure for each mode, throughout the model domain, as in all GLOMAP publications to date.

The routine UKCA_CALCNUCRATE has been updated to have an additional option for binary homogeneous nucleation of sulphuric acid and water. The scheme of Vehkamakki et al. (2002), which is applicable to both tropospheric and stratospheric conditions, has been added as an alternative to the Kulmala et al. (1998) parameterization, which is only appropriate for the troposphere. The switch i_bhn_method switches between the two schemes with a value of i_bhn_method_kulmala (equal to 1) and i_bhn_method_vekhamaki (equal to 2) for the Kulmala and Vehkamakki parameterizations, respectively. The switch i_bhn_method has been set to i_bhn_method_vekhamaki in UKCA_CALCNUCRATE and cannot be set at run time.

Two additional updates for stratospheric conditions are also included. Firstly, the calculation of water content in UKCA_VOLUME_MODE have also been modified to calculate the sulphuric acid weight percentage for stratospheric conditions from Carslaw et al. (1995), following code in the TOMCAT routine LACOMP, where the pressure is below 150 hPa. Secondly, the calculation of the particle density is amended in the stratosphere to switch to using the calculation of Martin et al. (2000), implemented via look-up table.

Note that although this code is included in version 8.2, the code has only been tested using vn7.3 at N48L60 resolution.

13.3.11 GLOMAP-mode options for boundary layer nucleation

As well as the two alternative binary nucleation schemes described above, there are additional switches to allow different approaches to allow the code to follow several alternative parameterizations for "boundary layer nucleation".

There are 3 boundary layer nucleation options controlled by the switch IBLN (which is set from the UKCA run-time switch I_MODE_BLN_PARAM_METHOD). The 3 different options (IBLN=1 to 3) follow those described in the Supplementary Material of Metzger et al. (2010) and those in Paasonen et al. (2010). For IBLN=1, traditional cluster activation approach is used, as in Spracklen et al. (2008) with the A value set at 0.5×10^{-6} s^{-1} and particles generated at 1.5nm dry diameter. For IBLN=2, the traditional kinetic nucleation parameterization (involving only sulphuric acid) is applied, as, for example in Spracklen et al. (2010), with $K = 0.4 \times 10^{-12}$ cm^3 s^{-1}, also generating particles at 1.5nm dry diameter. For IBLN=3, the organic-mediated nucleation rate from Metzger et al. (2010), is used, with nucleation rates at 1.5nm dry diameter then being determined by the concentrations of H_2SO_4 and SEC_ORG simulated by the model.

As well as the switch IBLN for the different boundary layer nucleation schemes the UKCA_CALCNUCRATE routine has been coded to allow the user to switch between different methods for implementing the chosen parameterization, and this is controlled via the switch I_NUC_METHOD. For I_NUC_METHOD=2, boundary layer nucleation is restricted to only occur within the boundary layer, whereas for I_NUC_METHOD=3, the parameterization is applied throughout the whole column (not recommended). This switch is set to 2 in UKCA_AERO_CTL and cannot be set at run time.

14 Coupling of chemistry and aerosols to the UM Radiation schemes

14.1 Radiatively active trace gases

The Edwards-Slingo radiation code includes the impact of the following radiatively active trace gases: H_2O; O_3; CO_2; CH_4; N_2O; CFC11; CFC12; CFC113; CFC114; HCFC22; HFC125 and HFC134A.

The values of CFC-11 and CFC-12 tracers also contain additions for other Cl species in the stratospheric chemistry scheme and these should not be selected for radiative forcing. Code to re-scale the CFCs to the correct value may be made available at a future version.

The Model always carries mixing ratios for water vapour and ozone as spatially varying fields. Water vapour is always prognostic. If neither UKCA or the Cariolle scheme is in use the ozone concentrations come from an ancillary file and the mixing ratios of other gases are held as uniform fields (unless the carbon cycle is used, when carbon dioxide is also held as a 3-dimensional field). The value of the mixing ratios of these uniform fields can be specified as fixed during a run or changing throughout a run using the run_radiation options for specification of trace gases.

When UKCA is on however, it is possible to couple the radiation code to the fields which are tracers in UKCA for any specific model configuration. For troposphere only models this will normally only be O_3 and CH_4 while stratospheric configurations will typically also allow N_2O, CFC11, CFC12, CFC113 and HCFC22 to be coupled to radiation.

The coupling is set up from Rose in the UKCA namespace, where there are switches for each of the gases which can be coupled to the radiation code. These control the following logicals:

l_ukca_rado3; l_ukca_radch4; l_ukca_radn2o; l_ukca_radf11; l_ukca_radf12; l_ukca_radf113; l_ukca_radf22

14.2 Direct effects of aerosols

The MODE aerosol scheme is very different from the CLASSIC aerosol schemes which have been used in the Unified Model so far. These differences impact the way aerosols interact with radiation to provide scattering and absorption of radiative fluxes (aerosol direct effect) and aerosol optical depth diagnostics. Additional code has been written in order to calculate the aerosol optical properties from MODE results, and this scheme is known as UKCA_RADAER. A summary of this scheme is provided below, further details are contained in a separate technical report (Bellouin (2010)).

14.2.1 Aerosol optical properties in the radiation scheme

The Unified Model radiation scheme divides the shortwave and longwave spectra into wavebands. Consequently, optical properties of atmosphere constituents, such as gases and aerosols, have to be integrated across those wavebands from the original monochromatic calculations. For aerosols, the radiation scheme requires the specific scattering and absorption coefficients, which describe the strength of aerosol scattering and absorption processes per unit aerosol mass (m^2 kg^{-1}), and the asymmetry parameter, which describes in a simplified way the angular dependence of the scattering (dimensionless). The specific scattering and absorption coefficients, and the asymmetry parameter, are hereafter referred to as the aerosol *optical properties*.

14.2.2 GLOMAP-mode aerosols

The GLOMAP-mode aerosol scheme not only simulates the dry aerosol mass, but also the mass of water attached to the aerosol, and the aerosol number concentrations. The total aerosol mass and number is distributed across 7 modes, characterised by their solubility and the range of particle sizes they cover. Each mode is made of a mixture of several aerosol chemical components, as listed in Table 22.

Modal aerosol size distributions are assumed to be lognormal, with the mean radius being interactively derived from the modal mass and number, and the standard deviation being prescribed. For the soluble modes it is 1.59 for the nucleation mode, 1.59 (Aitken); 1.4 (accumulation); and 2.0 (coarse). In the the insoluble modes it is 1.59 for Aitken and accumulation modes, and 2.0 for coarse mode.

The nucleation mode contains particles which are too small to be optically active and is therefore neglected by UKCA_RADAER.

Compared to CLASSIC, the GLOMAP-mode scheme introduces three important changes which are relevant to the radiation scheme:

1. The mean radius of the modal size distributions varies interactively;
2. The modal refractive index varies with the internal composition of the mode;
3. The amount of aerosol water in each soluble mode varies interactively.

Consequently, it is not possible to obtain the aerosol optical properties through offline calculations. They have to be computed at runtime, but doing monochromatic Mie calculations at runtime is expensive. Instead, UKCA_RADAER relies on pre-computed look-up tables of monochromatic optical properties, covering all realistic combinations of modal radii and refractive indices. As of version 2 of UKCA_RADAER, three sets of look-up tables are in use. Each set is made of two files, one for shortwave wavelengths, the other for longwave wavelengths. The first set, defined by environment variables UKCAACSW and UKCAACLW, is used to characterise Aitken and accumulation-mode aerosols. The second set, defined by environment variables UKCAANSW and UKCAANLW, is used specifically for soluble accumulation-mode aerosols, which can then be given a standard deviation different from that of other Aitken and accumulation mode aerosols. The third and final set is used to characterise coarse-mode aerosols and is identified by environment variables UKCACRSW and UKCACRLW.

At runtime, remaining tasks are:

1. to compute the modal refractive index out of the simulated chemical composition of each mode;
2. to obtain the monochromatic properties from the look-up tables at selected wavelengths within each shortwave and longwave wavebands;
3. to integrate across each waveband to obtain the waveband-averaged optical properties, which can be used by the radiation code.

In addition to the look-up tables, UKCA_RADAER requires some ancillary data describing the different aerosol components that can belong to a mode, as well as parameters for the integration across wavebands, such as the number and wavelength of the integration points. That file is expected to support all aerosol and water components listed in module *ukca_radaer_struct_mod* (9 components as of version 2 of UKCA_RADAER: ammonium sulphate, black carbon, organic carbon, sea-salt, mineral dust, secondary organic, ammonium nitrate, and sulphuric acid aerosols, and liquid water). The generation of the look up tables and external data required by UKCA_RADAER is described in a separate report (Bellouin (2010)).

14.2.3 Coupling with GLOMAP-mode

UKCA_RADAER requires input from GLOMAP-mode. The input needed resides in UKCA sections 34 (prognostic variables) and 38 (diagnostic variables). Input fields are:

- Aerosol number concentrations in each mode;
- Mass-mixing ratios of all aerosol components within each mode;
- Modal diameters for dry and, for soluble modes, wet aerosols;
- Modal density;
- Volume of each aerosol component in each mode and, for soluble modes, volume of aerosol water in the mode.

GLOMAP-mode data is acquired in *Atm_Step* and is stored into the UKCA_RADAER structure, which is defined by module *ukca_radaer_struct_mod*. When routine *Atm_Step* is first called, routine *ukca_radaer_init* initialises the structure. It lists the STASH items that are needed, depending on the configuration of GLOMAP-mode (active modes, active components within each mode). *ukca_radaer_init* exists in two version: the full version is compiled when section A34_1A is defined, i.e. when GLOMAP-mode is available. An error version is compiled when section A34_0A is defined and causes model failure, as UKCA_RADAER cannot be used without GLOMAP-mode.

The data itself is obtained by routine *ukca_radaer_get*. When it is first called, it scans D1 looking for the STASH items listed by *ukca_radaer_init*. Halo support is automatic, and the routine also checks that the input STASH fields have the expected dimensions and shape. If all required items are found, it transfers the GLOMAP-mode data to the UKCA_RADAER structure.

14.2.4 Within the radiation scheme

The UKCA_RADAER structure is passed down the calling tree to the radiation scheme, where relevant data is copied into local arrays, reshaped following the conventions used in the radiation scheme, as is also done for CLASSIC aerosols.

The actual interaction between GLOMAP-mode aerosols and radiation happens in routine *flux_calc*. First, the GLOMAP-mode data is processed by *ukca_radaer_prepare*. The routine computes the modal mass-mixing ratio by simply adding the component mass-mixing ratios together. It also converts the modal molecular concentrations to number concentrations (particles per m^{-3}).

The actual interaction can now take place. Waveband averaged optical properties of GLOMAP-mode aerosols are computed by routine *ukca_radaer_band_average*. For the purpose of interacting with radiation, sulphate aerosols are assumed to be in the form of ammonium sulphate throughout the atmosphere, unless logical switch L_UKCA_RADAER_SUSTRAT is activated, in which case sulphate aerosols take the optical properties of sulphuric acid in the stratosphere only. (The tropopause level is identified interactively by calling, if required, subroutine *tropin* in *atmos_physics1*.) Waveband-averaged properties are then transferred to routine *grey_extinction* and influence the calculation of atmospheric fluxes. In addition, modal optical depth diagnostics for GLOMAP-mode aerosols are computed, if requested, by *ukca_radaer_compute_aod* for each mode. This is only done in the longwave radiation routine in order to get Aerosol Optical Depth calculations in all gridboxes (shortwave radiation is only calculated on lit points). Again, whether sulphate aerosols in the stratosphere are in the form of ammonium sulphate or sulphuric acid is controlled by logical switch L_UKCA_RADAER_SUSTRAT. In RADAER v2 stratospheric AODs are also available for all aerosol modes as a STASH diagnostic. This is an addition to the existing AOD diagnostic that are calculated for the total atmospheric column. Results are transferred to routine *diagnostics_lw* for copy to STASH.

15 Indirect effects of aerosols

Atmospheric aerosols have a significant effect on the Earth's radiative balance both directly, by scattering and absorbing radiation, and indirectly, through their effects on cloud properties. A crucial link between aerosol and cloud is the ability of aerosols to act as cloud condensation nuclei (CCN) on which cloud droplets form, a process known as aerosol activation. An increase in the number of CCN leads to a greater number of smaller cloud droplets (for a cloud of constant liquid water content) with two main consequences: First, the larger surface area of a greater number of smaller droplets increases the cloud albedo (Twomey (1974)); Second, these smaller droplets are less efficient at coalescing to form raindrops which may increase the cloud amount and lifetime (Albrecht (1989)).

Aerosol activation is critically dependent on the size and composition of aerosols as well as the local supersaturation of water vapour. UKCA-Activate has been designed to explicitly represent these factors by coupling GLOMAP-mode, to a Köhler theory-based aerosol activation parameterisation (Abdul-Razzak and Ghan (2000)).

Variations in local vertical velocity have a significant effect on the maximum supersaturation achieved, and hence on the number of activated aerosols. In UKCA-Activate, the sub-grid-scale variability of updraught velocity is represented by a probability density function derived from the turbulent kinetic energy in the boundary layer. The cloud droplet number concentration (CDNC) throughout the vertical extent of warm clouds is approximated by the expected value of the number of aerosols that activate at cloud base, weighted by this pdf.

This diagnostic CDNC is then used to calculate the cloud droplet effective radius following Martin et al. (1994) which is passed to the Edwards-Slingo radiation code and hence used to determine the cloud albedo effect (first indirect aerosol effect).

UKCA is also coupled to the large-scale precipitation scheme due to the strong dependence on CDNC of the rate of autoconversion of cloud water to rain water (following the method of Tripoli and Cotton (1980)). This dependency permits estimation of the cloud lifetime effect and other secondary indirect aerosol effects in radiative flux perturbation calculations.

15.1 Logicals

- L_ukca_aie1: If TRUE, pass CDNC calculated by UKCA to the radiation scheme for effective radius calculation, thereby activating the first indirect aerosol effect. If FALSE, use fixed value of CDNC.

- L_ukca_aie2: If TRUE, pass CDNC calculated by UKCA to the large-scale precipitation scheme for use in autoconversion rate calculation, thereby activating the second indirect aerosol effect. If

FALSE, use fixed value of CDNC.

- L_ukca_arg_act: If TRUE, use Abdul-Razzak and Ghan (2000) aerosol activation scheme to calculate CDNC in UKCA-Activate. If FALSE, use Jones et al. (1994) empirical relation to estimate CDNC from GLOMAP-mode aerosol.
- L_ukca_sfix: If TRUE, provides diagnostics of potential CCN concentrations at fixed supersaturation, derived from GLOMAP-mode aerosol. Fixed values of supersaturation are currently set by hand in ukca_activate.f90 (as fractions, rather than percentages).

If L_ukca_aie1 and/or L_ukca_aie2 are TRUE, then CDNC calculated by UKCA are passed to the radiation and large-scale preceipitation schemes to allow the first and/or second indirect aerosol effects to be simulated. Additionally, if L_ukca_arg_act is TRUE, then UKCA-Activate is called at every time-step, from within UKCA, directly after the call to GLOMAP-mode. UKCA-Activate calls the Abdul-Razzak and Ghan (2000) aerosol activation to calculate CDNC from GLOMAP-mode aerosol.

However, if L_ukca_aie1 and/or L_ukca_aie2 are TRUE, but L_ukca_arg_act is FALSE, then UKCA uses the Jones et al. (1994) empirical relation to derive CDNC from the GLOMAP-mode aerosol. Either way, CDNC (in m^{-3}) as calculated by UKCA is output to D1 in section 34.

15.2 Inputs to UKCA-Activate

The following input fields are required from outside UKCA:

- pressure, temperature, specific humidity, saturated vapour pressure, air density, boundary layer turbulent kinetic energy, large-scale vertical velocity, liquid cloud fraction by volume, and cloud liquid water content.

Definitions of the aerosol modes and other aerosol properties are passed to UKCA-Activate in the call from UKCA. These are:

- Number of modes present.
- Number of chemical components possible in each mode.
- Molar mass of each possible component, in $\mathrm{kg\,mol^{-1}}$.
- Mass density of components, in $\mathrm{kg\,m^{-3}}$.
- Number of dissociating ions for soluble components.
- Geometric standard deviation of each mode (fixed).
- Logical definition of which modes are set.
- Logical definition of which components are set in each mode.

The following fields are calculated by GLOMAP-mode at each time step, stored in D1, and retrieved from there by UKCA-Activate:

- Number concentration of aerosol particles in each mode, in m^{-3}. (GLOMAP-mode generates a dimensionless number-equivalent volume mixing ratio which is similar to a volume mixing ratio but with 'particles per molecule of air' rather than 'molecules per molecule of air'. In UKCA-Activate, this is multiplied by the number density of air molecules, to obtain the number density of aerosol particles, as required by the activation scheme.)
- Mass mixing ratio of each component present in each mode, in kg (aerosol) / kg (air).
- Dry count median radius of each log-normal aerosol mode, in m, (calculated and stored by GLOMAP-mode as dry diameter).

15.3 UKCA-Activate

UKCA-Activate uses the Abdul-Razzak and Ghan (2000) aerosol activation scheme, which predicts number of activated aerosols, N_a, as a function of aerosol properties (size, number and composition), $a_i, i = 1...n$, vertical velocity, w, temperature, T, and pressure, p, such that it can be expressed as $N_\mathrm{a}(a_1, ..., a_n, T, p, w)$. The average number of activated aerosols within a grid-box is denoted as $\langle N_\mathrm{a} \rangle$.

15.3.1 Default sub-grid-scale vertical velocity configuration

The activation of aerosol to form cloud droplets is fundamentally dependent on the local supersaturation, as governed by the vertical velocity of the rising air. Typically, the large-scale vertical velocities resolved at the GCM grid-scale are small and it is the unresolved sub-grid-scale fluctuations which give rise to the updraughts associated with cloud formation. It is therefore necessary to account for this sub-grid-scale variability if aerosol activation is to be represented meaningfully in a GCM.

In the default configuration of UKCA-Activate, a probability density function (pdf) is used to represent the likely distribution of vertical velocity within each grid-box at each time-step. (It is assumed that the pdf has an explicit, continuous shape, $P(w)$.) The grid-box parameterisation is thus determined by calculating the expected value of the local parameterisation at each grid-box:

$$\langle N_\mathrm{a} \rangle = \frac{\int_0^\infty N_\mathrm{a}(a_1, ..., a_n, T, p, w) P(w) dw}{\int_0^\infty P(w) dw}. \tag{24}$$

Since aerosol activation does not occur in regions of downdraught, integration is only carried out for $w > 0$. By default, UKCA-Activate assumes a Gaussian distribution of probabilities across the grid-box, with mean $\bar{w}$ and standard deviation σ_w, i.e.

$$P(w) = \frac{1}{\sqrt{2\pi}\sigma_\mathrm{w}} \exp\left[-\left(\frac{(w - \bar{w})^2}{2\sigma_\mathrm{w}^2} \right) \right]. \tag{25}$$

Eqn. 24 is discretised over 20 equally-spaced bins of w extending out from $w = 0$ to $4\sigma_\mathrm{w}$. (A skewed Gaussian can be defined by setting the skewness parameter in ukca_activate.F90. Number of bins can be altered by changing the parameter nwbins in ukca_activate.F90. N.B. If nwbins is set to 1, a single value of vertical velocity is used instead of a pdf, and $N_\mathrm{d} = N_\mathrm{a}(w)$, where w is defined in the variable zvervel_max in ukca_activate.F90.)

Following the method of Ghan et al. (1997), the assumption is made that all sub-grid-scale variability in vertical velocity is due to turbulence. Within the scope of the boundary layer scheme (Lock and Edwards (2011)), σ_w is therefore diagnosed as

$$\sigma_{\rm w} = \max\left(\sqrt{\frac{2}{3}\mathrm{TKE}}, \sigma_{\rm w(min)}\right)\ \mathrm{m\,s^{-1}} \tag{26}$$

where TKE is the turbulent kinetic energy and $\sigma_{\rm w(min)}$ is a prescribed minimum value. Above the boundary layer, TKE is not currently diagnosed by the model, and $\sigma_{\rm w}$ must take on a fixed value, chosen here to be $\sigma_{\rm w(min)} = 0.1\mathrm{m\,s^{-1}}$.

In the absence of a cloud scheme with prognostic droplet number, the in-cloud droplet number concentration, $N_{\rm d}$, is simply set to the expected number of activated aerosols, $\langle N_{\rm a}\rangle$, for cloudy grid-boxes (those with liquid water content and cloud fraction > 0).

For vertically contiguous cloudy grid-boxes, it is assumed that $N_{\rm d}$ is constant with height and equivalent to $\langle N_{\rm a}\rangle$ at cloud base, throughout the depth of the cloud.

In the radiation scheme, the calculation of cloud droplet effective radius requires $N_{\rm d}^{-\frac{1}{3}}$, so the expected value of $N_{\rm a}^{-\frac{1}{3}}$ is also calculated, using

$$\left\langle N_{\rm a}^{-\frac{1}{3}}\right\rangle = \frac{\int_0^\infty (N_{\rm a}(w))^{-\frac{1}{3}}P(w)dw}{\int_0^\infty P(w)dw}, \tag{27}$$

(since $\left\langle N_{\rm a}^{-\frac{1}{3}}\right\rangle \neq \langle N_{\rm a}\rangle^{-\frac{1}{3}}$).

15.3.2 Outputs

Following these calculations, at the end of UKCA-Activate both $N_{\rm d}$ and $N_{\rm d}^{-\frac{1}{3}}$ are written to D1 as prognostic (but not transported) fields with STASH codes 34,162 and 34,163. A variety of optional diagnostics may also be output to section 38, see items 473 - 484.

15.4 Coupling to the rest of the UM

Following the method described in the previous section for UKCA_RADAER, a structure is used to retrieve UKCA CDNC from D1 and to pass it down from Atm_Step to where it is needed in the rest of the model. Module ukca_cdnc_mod defines the structure, ukca_cdnc_struct, which contains all of the variables needed to retrieve CDNC from D1.

Exactly as for UKCA_RADAER, this structure is initialised by ukca_cdnc_init the first time Atm_Step is called. The data is obtained by ukca_cdnc_get, which scans D1 looking for the STASH items listed by ukca_cdnc_init. Halo support is automatic, and the routine also checks that the input STASH fields have the expected dimensions and shape. If all required items are found, it transfers the CDNC calculated in UKCA to the UKCA_CDNC structure.

15.4.1 Coupling to radiation scheme

If L_ukca_aie1 is TRUE the CDNC values from UKCA (whether calculated by UKCA-Activate or from the empirical relation of Jones et al. (1994)) are passed to the radiation scheme and used in the calculation of cloud droplet effective radius ($r_{\rm e}$) in r2_re_mrf_umist-fill3a.F90.

15.4.2 Coupling to large-scale precipitation scheme

Similarly, if L_ukca_aie2 is TRUE the CDNC values from UKCA are passed to the large-scale precipitation scheme and used in the calculation of the rate and limit of autoconversion of liquid cloud water to rain water in lsp_autoc.F90, as described in UMDP26.

16 Lower Boundary Conditions

For UKCA stratospheric chemistry schemes (i.e. Standard Stratospheric and CheST) rather than having an emission into the long-lived gases, a lower boundary condition is specified (see table 26 for the species considered). Where this boundary condition comes from is defined by the `I_UKCA_SCENARIO` integer, the options of which are defined in table 25.

From the choice of `I_UKCA_SCENARIO` the UKCA routine `UKCA_SCENARIO_CTL` (which is called from `UKCA_MAIN1`) will then use the correct `UKCA_SCENARIO_...` routine. When using the `UKCA_SCENARIO_RCP` routine, used when `I_UKCA_SCENARIO=2`, the routine `TEST_SCENARIO_RCP` is provided, called from `TEST_SCENARIO_RCP_CTL`. These routines are used when the in-code logical `L_UKCA_TEST_SCENARIO_RCP=.TRUE.` (default `.FALSE.`). These routines will produce the files `Test_RCP_UKCA.dat` and `Test_RCP_Full.dat` (the latter file is only created if diagnostic messages are requested). This file contains the simulated daily values produced by the `UKCA_SCENARIO_RCP`, reading in the `UKCA_RCPFILE` file, simulating the years 1700–2550. This then allows the UKCA output to be checked against the values in the RCP file.

UKCA has the capability to use the UM-defined values of the radiative gases CH_4, N_2O, CFC11, CFC12, CFC113, CFC114, HCFC22, HFC125, and HFC134A as lower-boundary conditions for the Stratospheric and CheST chemistries (`I_UKCA_SCENARIO=0`), with CH_4 also being able to be taken for Tropospheric chemistry (`L_UKCA_PRESCRIBECH4=.TRUE.`). As well as this, the concentrations of CO_2, N_2 and H_2 may also be used by some tropospheric schemes as being constant throughout the whole atmosphere (rather than as a tracer, which may be altered by chemistry). In this case, the UM values can be taken as well. Other gases needed by UKCA can also be defined in the UKCA namespace of rose edit.

Table 26 gives a complete description of all trace gas values that UKCA reads in, which schemes these are used in, and where the value of these gases can be set. The corresponding code variable logical names are also included.

For the Stratospheric and CheST chemistries, if these values are prescribed for the lower boundary, this effectively means that a single year is re-run as a timeslice experiment. If these are not specified then UKCA will use its internal `UKCA_SCENARIO_WMOA1` routine which gives the lower boundary conditions from 1950-2100 following the SRES A1b scenario (as was used in CCMVal2). Specifying the values via Rose causes UKCA to use the `UKCA_SCENARIO_PRESCRIBED` subroutine instead. It should be noted that the `UKCA_SCENARIO_WMOA1` routine does not affect the values of these gases in the main UM code for radiative purposes. If this functionality is required then this will need to be added by the user (by a call to `UKCA_SCENARIO_CTL` from within `ATMOS_PHYSICS1` for those trace gases defined in the Rose radiation namespace).

The l_ukca_set_trace_gases logical allows some chemistry schemes using the Newton-Raphson solver (TropIsop, Strat, and Strattrop (CheST)) to take mass-mixing ratios from the radiation section of Rose (if these are defined as constant - `CT`), rather than the defaults of

$$\begin{aligned}
CO_2 &= 350.0 \times 10^{-6} \;\; \mathrm{kg}\,(CO_2)\,/\mathrm{kg}\,(\mathrm{air}) \\
H_2 &= 5.0 \times 10^{-7} \;\; \mathrm{kg}\,(H_2)\,/\mathrm{kg}\,(\mathrm{air}) \\
N_2 &= 0.78084 \;\; \mathrm{kg}\,(N_2)\,/\mathrm{kg}\,(\mathrm{air})
\end{aligned}$$

$$\mathrm{CH_4} \quad = \quad 1.76 \times 10^{-6} \;\; \mathrm{kg\,(CH_4)\,/kg\,(air)}\,.$$

It should be noted that if running with `I_UKCA_SCENARIO=0` then `L_UKCA_SET_TRACE_GASES` **must** be set to `.TRUE.`. It is also advisable that `L_UKCA_SET_TRACE_GASES=.TRUE.` for all schemes. While it is technically possible to run with `L_UKCA_SET_TRACE_GASES=.FALSE.` and `I_UKCA_SCENARIO=0` as the functionality provided by `L_UKCA_SET_TRACE_GASES` is unconnected with the lower boundary condition code, this is not advisable as the lower boundary condition value for H_2 will be set to the default (pre-industrial) value.

For the `L_UKCA_PRESCRIBECH4` logical, this just sets CH_4 for the UKCA tropospheric chemistries. It should be noted that the `I_UKCA_SCENARIO` integer (which **must** have a value for a stratospheric chemistry scheme such as Stratospheric or CheST) will over-ride the `L_UKCA_PRESCRIBECH4`, since `I_UKCA_SCENARIO` will take *all* trace gas values from the `UKCA_SCENARIO_CTL` routine, including CH_4. It is not possible to take some values from the radiation scheme settings and some from the `UKCA_SCENARIO_WMOA1` routine, and/or some from the `UKCA_SCENARIO_RCP` routine, i.e. all trace gas lower boundary condition concentrations can only come from one of the routines.

It is advisable that when using the `I_UKCA_SCENARIO=0` option, the user specify all gases in the Lower Boundary Conditions. If the user does not do this a warning is output and the code will use a value consistent with pre-industrial levels.

The lower boundary conditions are applied in `UKCA_EMISSION_CTL`, where the difference of the tracer concentration to the lower boundary condition is calculated as a 2D field, which is then treated as an emission. For species with concentrations less that the BC, this is positive, and for species with concentrations greater than the BC, this is negative. When the emissions routine is called, this results in enforcing the mixing ratio of the species at the surface.

Table 6: Advected tracers treated by the regional air quality chemistry scheme.

Item	Tracer name	STASH	Name	Dry	Wet	Emitted
1	O3	34001	O_3	Yes		
2	NO	34002	NO	Yes		Yes
3	NO3	34003	NO_3	Yes	Yes	
4	NO2	34004	NO_2	Yes		Yes
5	N2O5	34005	N_2O_5	Yes	Yes	
6	HO2NO2	34006	HO_2NO_2	Yes	Yes	
7	HONO2	34007	$HONO_2$	Yes	Yes	
8	H2O2	34008	H_2O_2	Yes	Yes	
9	CH4	34009	CH_4	Yes		Yes
10	CO	34010	CO	Yes		Yes
11	HCHO	34011	HCHO	Yes	Yes	Yes
12	MeOOH	34012	CH_3OOH	Yes	Yes	
13	C2H6	34014	C_2H_6			Yes
14	EtOOH	34015	C_2H_5OOH	Yes	Yes	
15	MeCHO	34016	CH_3CHO	Yes		Yes
16	PAN	34017	$CH_3O_3NO_2$	Yes		
17	C3H8	34018	C_3H_8	Yes		Yes
18	i-PrOOH	34020	i-C_2H_7OOH	Yes	Yes	
19	Me2CO	34022	CH_3COCH_3			Yes
20	O3S	34026	O_3 (Stratospheric)	Yes		
21	C5H8	34027	C_5H_8			Yes
22	ISOOH	34028	HOC_5H_8OOH			
23	ISON	34029	$(NO_3)C_4H_6CHO$			
24	MGLY	34034	CH_3-CO-CHO (methyl glyoxal)			
25	MVK	34039	CH_2=CH-CO-CH_3 (methyl vinyl ketone)			
26	MVKOOH	34040	$CH_3COCH(OH)CH_2OH$			
27	ORGNIT	34060	Lumped organic nitrates			
28	CH3OH	34069	CH_3OH (methanol)			Yes
29	H2	34070	H_2 (hydrogen)	Yes		Yes
30	RNC2H4	34090	$CH_2(NO_3)CHO$			
31	RNC3H6	34091	$CH_3CH(NO_3)CHO$			
32	C2H4	34092	C_2H_4			Yes
33	C3H6	34093	C_3H_6			Yes
34	C4H10	34094	C_4H_{10}			Yes
35	C4H9OOH	34095	C_4H_9OOH			
36	MEK	34096	CH_3-CO-C_2H_5			
37	TOLUENE	34097	Toluene			Yes
38	MEMALD	34098	CH_3-CO-CH=CH-CHO			
39	GLYOXAL	34099	Glyoxal			
40	oXYLENE	34100	o-Xylene			Yes

Table 7: Non-advected tracers treated by the regional air quality chemistry scheme.

Item	Tracer name	STASH	Name	Dry	Wet	Emitted
1	O3P	34151	$O(^3P)$			
2	O1D	34152	$O(^1D)$			
3	OH	34153	OH			
4	HO2	34154	HO_2		Yes	
5	MeOO	34155	CH_3O_2		Yes	
6	EtOO	34156	$C_2H_5O_2$			
7	MeCO3	34157	CH_3COO_2			
8	s-BuOO	34158	s-$C_4H_9O_2$			
9	i-PrOO	34159	i-$C_3H_7O_2$			
10	MeCOCH2OO	34160	CH_3-CO-CH_2O_2			
11	MEKO2	34161	$CH_3COCH(O_2)CH_3$			
12	HOC2H4O2	34162	$CH_2O_2CH_2OH$			
13	HOC3H6O2	34163	$CH_3CHO_2CH_2OH$			
14	OXYL1	34164	$C_6H_5CH_2O_2$			
15	MEMALD1	34165	$CHOCH(OH)CO_2CH_3CHO$			
16	HOIPO2	34166	$HOC_5H_8O_2$			
17	HOMVKO2	34167	$CH_3COCH(O_2)CH_2OH$			
18	TOLP1	34168	$HOC_6H_5CH3O_2$			

Table 8: Advected tracers and diagnostic species treated by the stratospheric chemistry scheme. The diagnostic species are NO_2, BrO, and HCl.

	STASH name	STASH	UKCA Species	Dry	Wet	Emitted/Lower BC
1	Specific Humidity	10	q			
2	O3	34001	O_3	Yes		
3	NO	34002	NO			Emitted
4	NO3	34003	NO_3	Yes	Yes	
5	N2O5	34005	N_2O_5	Yes	Yes	
6	HO2NO2	34006	HO_2NO_2	Yes	Yes	
7	HONO2	34007	$HONO_2$	Yes	Yes	
8	H2O2	34008	H_2O_2	Yes	Yes	
9	CH4	34009	CH_4			Lower BC
10	CO	34010	CO	Yes		Emitted
11	HCHO	34011	HCHO	Yes	Yes	Emitted
12	MeOOH	34012	CH_3OOH	Yes	Yes	
13	Cl	34041	Cl			
14	ClO	34042	ClO			
15	Cl2O2	34043	Cl_2O_2			
16	OClO	34044	OClO			
17	Br	34045	Br			
18	BrCl	34047	BrCl			
19	BrONO2	34048	$BrONO_2$		Yes	
20	N2O	34049	N_2O			Lower BC
21	HOCl	34051	HOCl		Yes	
22	HBr	34052	HBr		Yes	
23	HOBr	34053	HOBr		Yes	
24	ClONO2	34054	$ClONO_2$		Yes	
25	CFCl3	34055	$CFCl_3$			Lower BC
26	CF2Cl2	34056	CF_2Cl_2			Lower BC
27	MeBr	34057	CH_3Br			Lower BC
28	N	34058	N			
29	O(3P)	34059	$O(^3P)$			
30	H2	34070	H_2			Lower BC
31	H	34080	H			
32	OH	34081	OH			
33	HO2	34082	HO_2		Yes	
34	MeOO	34083	CH_3O_2		Yes	
35	Lumped N	34098				
36	Lumped Br	34099				
37	Lumped Cl	34100				
38	PASSIVE O3	34149	Passive O3			
39	AGE OF AIR	34150	Age of Air			
35	NO2	34153	NO_2	Yes		
36	BrO	34154	BrO			
37	HCl	34155	HCl		Yes	

Table 10: Sulphur and monoterpene oxidation scheme for Newton-Raphson tropospheric chemistry. References are: 1) Pham et al. (1995); 2) Kreidenweis et al. (2003); and 3) IUPAC Subcommittee for Gas Kinetic Data Evaluation for Atmospheric Chemistry). Monoterpene is treated as alpha-pinene, with 4) secondary organic product formed with the product yield shown (Spracklen et al. (2006)).

Reaction	Reference
Gas phase reactions	
$DMS + OH \rightarrow SO_2 + CH_3O_2 + HCHO$	1
$DMS + OH \rightarrow 0.6SO_2 + 0.4DMSO + CH_3O_2$	1
$DMS + NO_3 \rightarrow SO_2 + HNO_3 + CH_3O_2 + HCHO$	1
$DMSO + OH \rightarrow 0.6SO_2 + 0.4MSA$	1
$CS_2 + OH \rightarrow SO_2 + COS$	1
$H_2S + OH \rightarrow SO_2$	1
$COS + OH \rightarrow SO_2$	1
$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	1
$MONOTERPENE + OH \rightarrow 0.13SEC\_ORG$	3,4
$MONOTERPENE + O3 \rightarrow 0.13SEC\_ORG$	3,4
$MONOTERPENE + NO3 \rightarrow 0.13SEC\_ORG$	3,4
Aqueous phase reactions	
$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-}$	2
$HSO_3^- + O_3 \rightarrow SO_4^{2-}$	2
$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	2

Table 11: Additional advected tracers available for the tropospheric and stratospheric aerosol chemistry schemes.

Item	STASH Name	STASH item	Species name	Dry	Wet	Emitted
1	DMS	34071	CH_3SCH_3			Yes
2	SO2	34072	SO_2	Yes	Yes	Yes
3	H2SO4	34073	H_2SO_4			
4	MSA	34074	CH_3SO_3H	Yes		
6	DMSO	34075	CH_3SOCH_3	Yes	Yes	
5	NH3	34076	NH_3	Yes	Yes	Yes
7	CS2	34077	CS_2			Yes
8	COS	34078	COS			Yes
9	H2S	34079	H_2S			Yes
10	Monoterp	34091	$C_{10}H_{16}$	Yes		Yes
11	Sec_Org	34092		Yes	Yes	
12	SO3	34094	SO_3	Yes	Yes	

Reaction	Rate
$DMS + OH \rightarrow CH_3SO_2$	k_1
$DMS + OH \rightarrow CH_3SO_2$	$0.9 \times k_2$
$DMS + OH \rightarrow MSA$	$0.1 \times k_2$
$DMS + NO_3 \rightarrow CH_3SO_2$	k_7
$CH_3SO_2 \rightarrow SO_2 + CH_3$	k_3
$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	k_4
$CH_3SO_2 + NO_2 \rightarrow CH_3SO_3$	k_8
$CH_3SO_3 + HO_2 \rightarrow MSA$	k_5
$CH_3SO_3 \rightarrow SO_3 + CH_3$	k_6

Table 12: Simplified DMS oxidation scheme.

Rate	Value	Reference
k_1	$1.12 \times 10^{-11} exp(-250/T)$	(1)
k_2	$(9.3 \times 10^{-39} exp(5270/T)[O_2])/$	
	$(1 + (7.4 \times 10^{-29} exp(5610/T)[O_2]))$	(1)
k_3	100.0	(2)
k_4	6.3×10^{-13}	(2)
k_5	5.0×10^{-11}	(2)
k_6	1.2×10^{-3}	(2)
k_7	$1.9 \times 10^{-3} exp(-520/T)$	(1)
k_8	2.2×10^{-11}	(2)

Table 13: Rate coefficients used in the parameterised DMS mechanism
(1) IUPAC Subcommittee for Gas Kinetic Data Evaluation for Atmospheric Chemistry, (2) Karl et al. (2007)

Reaction	Reference
$SO_2 + O_3 \rightarrow SO_3$	(1,2)
$SO_3 + H_2O \rightarrow H_2SO_4 + H_2O$	(1)
$COS + O(^3P) \rightarrow CO + SO_2$	(1,2)
$H_2S + O(^3P) \rightarrow OH + SO_2$	(1,2)
$CS_2 + O(^3P) \rightarrow COS + SO_2 + CO$	(1,2)
$DMS + O(^3P) \rightarrow SO_2$	(1,2)
$SO_2 + OH + M \rightarrow SO_3 + HO_2 + M$	(2)
$CS_2 + h\nu \rightarrow COS + SO_2$	(2)
$COS + h\nu \rightarrow CO + SO_2$	(2)
$H_2SO_4 + h\nu \rightarrow SO_3 + OH$	(2)
$SO3 + h\nu \rightarrow SO_2 + O(^3P)$	(2)

Table 14: Stratospheric sulphur chemistry scheme (extra or modified reactions only). Sources: 1) JPL (2006); 2) Weisenstein et al. (1997)

Table 15: Chemical array dimensions

Name	Description
jpctr	No. of chemical tracers
jpspec	No. of chemical species
jpbk	No. of bimolecular reactions
jptk	No. of termolecular reactions
jpjj	No. of photolytic reactions
jphk	No. of heterogeneous reactions
jpnr	No. of reactions
jpdd	No. of dry deposited species
jpdw	No. of wet deposited species

Table 16: Photolysis schemes

Number	Description
0	No photolysis
1	2D photolysis
2	Fast-J
3	Fast-JX

Table 17: Species treated by the interactive dry deposition scheme.

Model Name	Formula
O3	O_3
NO	NO
NO2	NO_2
NO3	NO_3
N2O5	N_2O_5
HONO2	HNO_3
HONO	HONO
ISON	
H2SO4	H_2O_4
H2O2	H_2O_2
H2	H_2
CH3OOH	CH_3OOH
HACET	
ROOH	Other organic peroxides
PAN	
PPAN	
MPAN	
CO	CO
CH4	CH_4
NH3	NH_3
H2	H_2
SO2	SO_2
DMSO	
MSA	
OnitU	
SEC_ORG	Any other secondary organics
ORGNIT	Organic nitrogen

Table 18: Emissions species required by UKCA configurations. Unless otherwise specified, mass is specified as that of the species concerned.

Emission Species	Units	Std Trop	Trop-Isop	RAQ Chem	Strat Chem	Strat+ Trop
NOx Surface Emissions	kg(NO2)/m^2/s	Y	Y	Y	Y	Y
CH4 Surface Emissions	kg(CH4)/m^2/s	Y	Y	Y	Y	Y
CO Surface Emissions	kg/m^2/s	Y	Y	Y	Y	Y
HCHO Surface Emissions	kg/m^2/s	Y	Y	Y	Y	Y
C2H6 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
C3H8 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
CH3COCH3 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
CH3CHO Surface Emissions	kg/m^2/s	Y	Y	Y		Y
C5H8 (Isop) Surface Emiss	kg(C)/m^2/s		Y	Y		Y
H2 Surface Emissions	kg/m^2/s			Y		
C4H10 Surface Emissions	kg/m^2/s			Y		
C2H4 Surface Emissions	kg/m^2/s			Y		
C3H6 Surface Emissions	kg/m^2/s			Y		
Toluene Surface Emissions	kg/m^2/s			Y		
o-xylene Surface Emissions	kg/m^2/s			Y		
CH3OH Surface Emissions	kg(C)/m^2/s			Y		
NOx Aircraft Emissions (3D)	kg(NO2)/m^2/s	Y	Y	Y	Y	Y
If using Aerosol Chem						
Monoterpene Surface Emiss	kg(C)/m^2/s	Y	Y			Y
NVOC Surface Emiss	kg(C)/m^2/s		Y			Y
SO2 Surface Emissions	kg(S)/m^2/s	Y	Y		Y	Y
DMS Surf Emiss (Land,ocean)	kg(S)/m^2/s	Y	Y		Y	Y
NH3 Surface Emissions	kg/m^2/s	Y	Y			Y
SO2 High (Ind,forest,ship)	kg(S)/m^2/s	Y	Y		Y	Y
SO2 Volcanic Emissions (3D)	kg(S)/m^2/s	Y	Y		Y	Y
for GLOMAP-mode (if using 5-mode setup)						
BC Fossil Fuel Emiss	kg(C)/m^2/s	Y	Y			Y
OC Fossil Fuel Emiss	kg(C)/m^2/s	Y	Y			Y
BC Biofuel Emissions	kg(C)/m^2/s	Y	Y			Y
OC Biofuel Emissions	kg(C)/m^2/s	Y	Y			Y
BC Biomass burn Emiss (3D)	kg(C)/m^2/s	Y	Y			Y
OC Biomass burn Emiss (3D)	kg(C)/m^2/s	Y	Y			Y
Online Emissions						
CH4 Wetland Emiss (in LSH - Optional)	kg(C)/m^2/s	Y	Y	Y	Y	Y
Lightning NOx (in UKCA)	kg(NO2)/kg(air)/cell/s	Y	Y	Y	Y	Y
Sea-Salt Emiss (in GLOMAP-mode)	number/m^2/s	Y	Y		Y	Y

Table 20: Item numbers for new emission diagnostics present in the RAQ chemistry scheme as indicated in the module GET_EMDIAG_STASH_MOD.

Emission field (in em_chem_spec)	Item number (in Sect. 50)
'NO '	156
'CH4 '	157
'CO '	158
'HCHO '	159
'C2H6 '	160
'C3H8 '	161
'Me2CO '	162
'MeCHO '	163
'C5H8 '	164
'C4H10 '	165
'C2H4 '	166
'C3H6 '	167
'TOLUENE '	168
'oXYLENE '	169
'CH3OH '	170
'H2 '	171
'NO_aircrft'	172

Table 21: Correspondence between metadata attributes in NetCDF emission files and variables in the emissions structure of the UKCA code. See also notes in Table 19.

Attribute in NetCDF files	Corresponding name in emissions structure within the UKCA code
name	emissions(:)%var_name
standard_name	emissions(:)%std_name
long_name	emissions(:)%lng_name
tracer_name	emissions(:)%tracer_name
units	emissions(:)%units
hourly_scaling	emissions(:)%hourly_fact
daily_scaling	emissions(:)%daily_fact
vertical_scaling	emissions(:)%vert_fact
lowest_level	emissions(:)%lowest_lev
highest_level	emissions(:)%highest_lev
update_freq_in_hours (global)	emissions(:)%update_freq
emission_type (global)	emissions(:)%update_type

Table 22: The seven modes in the GLOMAP-mode aerosol scheme, their size ranges and their components. Components are sulphate (SU), black carbon (BC), organic carbon (OC), sea salt (SS) and dust (DU). $\overline{r}$ is the geometric mean radius (nm) of aerosol particles.

Mode name	Size range (nm)	Composition	Solubility	Mode width
Nucleation soluble	$\overline{r} < 5$	SU, OC	Yes	1.59
Aitken soluble	$5 < \overline{r} < 50$	SU, BC, OC	Yes	1.59
Aitken insoluble		BC, OC	No	1.59
Accumulation soluble	$50 < \overline{r} < 500$	SU, BC, OC, SS, DU	Yes	1.40
Accumulation insoluble		DU	No	1.59
Coarse soluble	$500 < \overline{r}$	SU, BC, OC, SS, DU	Yes	2.0
Coarse insoluble		DU	No	2.0

Table 23: Advected tracers treated by the MODE aerosol scheme (Soluble Modes).

Item	Tracer name	STASH	Name	MS1	MS2	MS4	MS8
			Nucleation Mode (Soluble)				
1	ND_Nuc_SOL	34101	Number Density	X	X	X	X
2	Nuc_SOL_SU	34102	Sulphate MMR	X	X	X	X
3	Nuc_SOL_OC	34126	Organic Carbon MMR		X		X
4	Nuc_SOL_OZ	34128	Organic Carbon 2 MMR			X	
			Aitken Mode (Soluble)				
5	ND_Ait_SOL	34103	Number Density	X	X	X	X
6	Ait_SOL_SU	34104	Sulphate MMR	X	X	X	X
7	Ait_SOL_BC	34105	Black Carbon MMR		X	X	X
8	Ait_SOL_BC	34106	Organic Carbon MMR		X	X	X
9	Ait_SOL_SS	34127	Sea Salt MMR				
10	Ait_SOL_OZ	34129	Organic Carbon 2 MMR			X	
			Accumulation Mode (Soluble)				
11	ND_Acc_Sol	34107	Number Density	X	X	X	X
12	Acc_SOL_SU	34108	Sulphate MMR	X	X	X	X
13	Acc_SOL_BC	34109	Black Carbon MMR		X	X	X
14	Acc_SOL_OC	34110	Organic Carbon MMR		X	X	X
15	Acc_SOL_SS	34111	Sea Salt MMR	X	X	X	X
16	Acc_SOL_DU	34112	Dust MMR				X
17	Acc_SOL_OZ	34130	Organic Carbon 2 MMR			X	
			Coarse Mode (Soluble)				
18	ND_Cor_SOL	34113	Number Density	X	X	X	X
19	Cor_SOL_SU	34114	Sulphate MMR	X	X	X	X
20	Cor_SOL_BC	34115	Black Carbon MMR		X	X	X
21	Cor_SOL_OC	34116	Organic Carbon MMR		X	X	X
22	Cor_SOL_SS	34117	Sea Salt MMR	X	X	X	X
23	Cor_SOL_DU	34118	Dust MMR				X
24	Cor_SOL_OZ	34131	Organic Carbon 2 MMR			X	

Table 24: Advected tracers treated by the MODE aerosol scheme (Insoluble Modes).

Item	Tracer name	STASH	Name	MS1	MS2	MS4	MS8
Aitken Mode (Insoluble)							
25	ND_Ait_INS	34119	Number Density		X	X	X
26	Ait_INS_BC	34120	Black Carbon MMR		X	X	X
27	Ait_INS_OC	34121	Organic Carbon MMR		X	X	X
Accumulation Mode (Soluble)							
28	ND_Acc_INS	34122	Number Density				X
29	Acc_INS_DU	34123	Dust MMR				X
Coarse Mode (Insoluble)							
30	ND_Cor_INS	34124	Number Density				X
31	Cor_INS_DU	34125	Dust MMR				X

Table 25: Options provided by `I_UKCA_SCENARIO`.

Value	Further variables required	Specification of Lower BCs
0	None	Values are taken from Rose, either from where the radiative trace gases are specified, or the UKCA section. This uses the `UKCA_SCENARIO_PRESCRIBED` routine.
1	None	Values are taken from the `UKCA_SCENARIO_WMOA1` routine, which contains values from the SRES A1b scenario. This option can only be used for model years between 1950–2100.
2	`UKCA_RCPDIR` `UKCA_RCPFILE`	This option uses the `UKCA_SCENARIO_RCP` routine which reads in values from the CMIP5 website `http://cmip-pcmdi.llnl.gov/cmip5/forcing.html`. It may be necessary to run `dos2unix` on these files.

Table 26: Definition of UKCA Lower Boundary Conditions for chemical species. NOTE: these values are only taken from the radiation scheme settings when the logicals are set to `.TRUE.` or when `I_UKCA_SCENARIO=0`.

Use	Scheme	Species	Internal Variable	GUI location	UKCA Control Parameter
Constant	All	CO_2	`CO2_MMR`	Main radiation namespace	`L_UKCA_SET_TRACE_GASES`
Constant	All	O_2	`O2MMR`	Main radiation namespace	`L_UKCA_SET_TRACE_GASES`
Constant	All	N_2	`ukca_N2MMR`	UKCA namespace	`L_UKCA_SET_TRACE_GASES`
Constant	StdTrop, TropIsop	H_2	`ukca_H2MMR`	UKCA namespace	`L_UKCA_SET_TRACE_GASES`
Lower BC	StdTrop, RAQ, TropIsop	CH_4	`CH4MMR`	Main radiation namespace	`L_UKCA_PRESCRIBECH4`
Lower BC	Strat, CheST	CH_4	`CH4MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	N_2O	`N2OMMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CFC-11	`C11MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CFC-12	`C12MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CFC-113	`C113MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CFC-114	`C114MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	HCFC-22	`HCFC22MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	HFC-125	`HFC125MMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	HFC-134a	`HFC134AMMR`	Main radiation namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CH_3Br (MeBr)	`ukca_MeBrMMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CH_3Cl (MeCl)	`ukca_MeClMMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CH_2Br_2	`ukca_CH2Br2MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	H_2	`ukca_H2MMR`	UKCA namespace	`L_UKCA_SET_TRACE_GASES`
Lower BC	Strat, CheST	N_2	`ukca_N2MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CFC-115	`ukca_CFC115MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CCl_4	`ukca_CCl4MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	CH_3CCl_3 (MeCCl3)	`ukca_MeCCl3MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	HCFC-141b	`ukca_HCFC141bMMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	HCFC-142b	`ukca_HCFC142bMMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	Halon 1211 (H1211)	`ukca_H1211MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	Halon 1202 (H1202)	`ukca_H1202MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	Halon 1301 (H1301)	`ukca_H1301MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Strat, CheST	Halon 2402 (H2402)	`ukca_H2402MMR`	UKCA namespace	`I_UKCA_SCENARIO`
Lower BC	Stratospheric Aerosol	COS	`ukca_COSMMR`	UKCA namespace	`I_UKCA_SCENARIO`

17 Lateral boundary conditions (LBCs)

Code is been available to write and read in lateral boundary conditions (LBCs) which include UCKA tracers in addition to the other prognostic variables normally used in limited area models. This section is simply a description of how to enable this functionality for UKCA. For more details on the formulation of lateral boundary conditions please see UMDP C71 (Gardner and Burton (2006)).

17.1 Generation of LBCs

To use MakeBC to generate LBCs from the MetUM output after a model run, ensure that you have all the requried model ouput going to a fields file and then run MakeBC. See the instructions in UMDP F54 (Green and Whitehouse (2010)).

17.2 Using LBCs

Set up the input of the LBCs as for a normal LAM. The UKCA tracers to be read in are set using the entry boxes on the UKCA namespace. This table will only be active if your model is a limited area model not a global model.

Ensure that the UKCA tracer LBC inputs which you choose (by setting the value in the boxes to 1) match the fields present in the LBC file you are reading in or the model will fail on the first timestep. If a LBC for a tracer is not present, this means it will be treated as if there is no source of the tracer outside your model i.e. the LBC is effectively zero.

17.3 STASH codes for UKCA LBCs

Unlike for standard LBC fields all the LBCs for UKCA tracers are in section 37. The lateral boundary values for tracer 1 are stored in STASH code 37001 etc. The LBC tendencies calculated by the LBC routines for tracer 1 are held in STASH code 37257 etc for consistency with section 31 LBCs.

18 Diagnostics

18.1 Driving diagnostics

The diagnostics required to drive UKCA are described in section 3, and are listed in table 30.

18.2 Standard output diagnostics scheme for ASAD

A diagnostics scheme, primarily for use with the ASAD package, has been included in this release. These diagnostics are held in two routines `ASAD_CHEM_FLUX_DIAGS` and `ASAD_FLUX_DAT`, both of which are modules. Currently, the routines held in `ASAD_CHEM_FLUX_DIAGS` allow for the diagnostics listed in Tabel 27.

The three- and one-letter codes are used in `ASAD_FLUX_DAT` using the derived-type `ASAD_FLUX_DEFN` to define a diagnostics, e.g.

```
ASAD_FLUX_DEFN(’RXN’,50001,’B’,.TRUE.,0,4, &
(/’HO2       ’,’NO        ’/), &
(/’OH        ’,’NO2       ’,’          ’,’          ’/))
```

Table 27: UKCA/ASAD Diagnostics Package.

Diagnostic	Units	Three-letter code	One-letter codes
Reaction Flux	mole/gridcell/s	RXN	B = Bimolecular T = Termolecular J = Photolysis H = Heterogeneous
Deposition Flux	mole/gridcell/s	DEP	D = Dry Deposition W = Wet Deposition
Emission Flux	mole/gridcell/s	EMS	S = Surface Emissions A = Aircraft Emissions V = Volcanic Emissions T = 3D SO2 Emissions L = Lightning Emissions
Stratosphere-Troposphere Exchange	mole/gridcell/s	STE	X = One-letter code not required
Air Mass	kg	MAS	X = One-letter code not required
Chemical Tendency	mole/gridcell/s	NET	X = One-letter code not required
Polar Stratospheric Cloud Fraction	No Units	PSC	1 = PSC Type 1 2 = PSC Type 2
Tropospheric Mask Fraction	No Units	TPM	X = One-letter code not required
Tracer Concentration	kg(Tracer)/kg(air)	OUT	X = One-letter code not required
Lightning Nitrogen	molecules	LIN	X = One-letter code not required
Lightning Flash Rate	flashes/gridcell/s	LGT	T = Total Flashes G = Cloud-to-Ground Flashes C = Cloud-to-Cloud Flashes

where `ASAD_FLUX_DEFN` is defined as

```
TYPE ASAD_FLUX_DEFN
CHARACTER(LEN=3) :: diag_type
INTEGER :: stash_number
CHARACTER(LEN=1) :: rxn_type
LOGICAL :: tropospheric_mask
INTEGER :: rxn_location
INTEGER :: num_species
CHARACTER(LEN=10) :: reactants(2)
CHARACTER(LEN=10) :: products(4)
ENDTYPE ASAD_FLUX_DEFN
```

The meanings of these fields is defined in Table 28.

Within `ASAD_FLUX_DAT` a standard set of diagnostics has been coded for general use (see Appendix D).

It is relatively straight-forward to add new code (for a completely new diagnostic) to `ASAD_CHEM_FLUX_DIAGS`. This requires:

Table 28: Explanation of ASAD_FLUX_DEFN.

Variable	Meaning
diag_type	The diagnostic requested, as chosen by the three-letter code from Table 27.
stash_number	The 5-digit STASH code which the diagnostic will be output through.
rxn_type	The sub-type within the diagnostic, defined by the one-letter code from Table 27.
tropospheric_mask	A logical which is set to `.TRUE.` if this diagnostic is only to have values in the troposphere (and zero above) and `.FALSE.` if the diagnostic will have values over the whole domain.
rxn_location	This is only used for reactions where the reactants and products are the same in more than one reaction, but these reactions have different rates. Setting this to 0 will take the first found in the list of reactions, setting to any other number will take that number in the list.
num_species	The total number of species in the diagnostic (reactants + products).
reactants(2)	If a reaction, both elements will contain a species, otherwise only the first element will be used.
products(4)	The products of the reaction. Only used if requesting a reaction flux.

1. The appropriate three- and one-letter codes to be defined and made public
2. The creation of a logical which will turn on the diagnostic in the UKCA code (e.g. `L_ASAD_USE_STE`). These are set to `.FALSE.` initially and turned on by the code in `ASAD_INIT_CHEMDIAG`. This needs to be made public.
3. The diagnostic needs to be added to the `CASE` statement in `ASAD_INIT_CHEMDIAG`. This needs to turn on the diagnostics logical, and set the two logicals in the diagnostics derived type; `%CAN_DEALLOCATE` which controls whether the diagnostic can be deallocated at the end of `UKCA_MAIN1`, and `%OUTPUT_ON_CHEM_TSTEP` which checks to see if the diagnostic is requested at all times or only at chemical timesteps.
4. The diagnostic routine needs to be added to the module held in `ASAD_CHEM_FLUX_DIAGS`, added to the interface block, and made public.
5. The call to the diagnostic needs to be protected by its own logical and the logical `L_ASAD_USE_CHEM_DIAGS`.
6. The diagnostic needs to be added to the end of `ASAD_FLUX_DAT` with the `ASAD_CHEMICAL_FLUXES` array incremented accordingly.
7. A STASHmaster file needs to be created matching the STASH code(s) in the new diagnostic.

8. If this diagnostic is accepted as standard, the diagnostic appendix (Appendix D) in the UKCA UMDP (this document) will need to be updated.

For these standard diagnostics, these will be output through STASH when requested. For reaction fluxes it is important to only output values on chemical timesteps (currently 1 hour) to prevent sampling issues. This is protected by the `%OUTPUT_ON_CHEM_TSTEP` logical in the derrived type.

19 Control features

UKCA has several different chemistry schemes and includes the GLOMAP-mode aerosol scheme which can be configured in many ways. The control of the model is done using rose edit, and the help buttons of this interface provide additional information on how to set up UKCA. Note that options which are not valid for a specific UKCA set up will not be visible. For example if UKCA is turned off (l_ukca = .FALSE.) no other UKCA related items will be visible in rose edit.

The control variables are transferred into the code via the RUN_UKCA namelist. The RUN_UKCA namelist is located in the UKCA module ukca_option_mod. Table 32 shows the control logicals, and table 33 shows the remaining control variables. Table 34 shows logicals which are currently set in the code, together with their state.

The UKCA namespace has a series of sections which select features of the model. Some options which can be set here include:

- The main logical to turn UKCA on or off.
- The chemical scheme and optional variables affecting the Backward-Euler solver. The option "only age of air", which does not include chemistry, can be selected from Rose. Age of air will also be automatically calculated when running stratospheric chemistry schemes.
- Interactive emissions, such as CH4 emissions from wetlands.
- Tropospheric and stratospheric chemistry options.
- The type of photolysis scheme. See the descriptions of these schemes elsewhere in this document and the help for more information.
- Lower boundary conditions for the model so that a scenario based on prescribed surface concentrations may be followed. Note that this option also fills species which are set as global constants. Species which may be set in this way are CO_2, H_2, N_2 and CH_4.
- Coupling with other parts of the model. This includes radiatively active trace gases and aerosols and the interactive dry deposition scheme.
- The main switch for the GLOMAP-mode aerosol and choices for this scheme. Select "sulphate and sea-salt components in 4 soluble modes" when using stratospheric (Strat, Strattrop (CheST)) chemistry, and "sulphate, sea-salt, black carbon (BC) and organic carbon (OC) components in 4 soluble modes and 1 insoluble mode" when using tropospheric chemistry.
- New emission system in UKCA (NetCDF)

A Calling Tree

The complete calling tree of the UM can be accessed from the Unified Model web page (see under ”Browse Source”). Figure 2 shows a brief listing of the main routines.

```
UKCA_MAIN
|
+---UKCA_CHEM1_INIT (initialise chemical scheme)
|
+---UKCA_SETD1DEFS (select prognostics and diagnostics required by UKCA)
|
+---GETD1FLDS (read in D1 fields and transform)
|
+---UKCA_FASTJ/UKCA_FASTJX (call photol)
|
+---UKCA_EMISSION_CTL
|   |
|   +---TR_MIX (do boundary layer mixing and add in surface emissions)
|   |
|   +---LIGHT_CTL (calculate lightning emissions)
|   |
|   +---TRSRCE (add in 3-dimensional emissions)
|   |
|   +--UKCA_VOLCANIC SO2 (add volcanic emissions to stratosphere)
|
+---UKCA_CHEMISTRY_CTL
|   |
|   +-DDEPCTL(calculate dry deposition rates)
|   |
|   +-WDEPRT (calculate wet deposition rates)
|   |
|   +-ASAD_CDRIVE (call ASAD chemical solver)
|   |
|   +-UKCA_STRATF (calculate upper boundary conditions)
|
+---UKCA_AERO_CTL (call GLOMAP-mode aerosol model)
|
+---UKCA_ACTIVATE (call ACTIVATE model for CDNC)
|
+---PUTD1FLDS (put prognostic fields into D1)
|
+---STASH (store diagnostics fields)
```

Figure 2: UKCA Outline calling tree

B Driving Fields

Table 29 shows the prognostic MetUM fields used to drive UKCA and table 30 shows the diagnostic driving fields. These tables also include the name of the variable in the ukca_main1 top level subroutine and some information on how the variable is used. Table 31 shows the fields which are optionally output from UKCA and used in other locations. Which of these are available from UKCA and which are used by other sections will depend on the configuration of UKCA and the settings of logical control variables.

Table 29: Prognostic driving fields used by UKCA.

Sect	Item	Description	UKCA variable name	Where used
0	004	Theta	theta	widely
0	009	soil moisture	soil_layer_moisture	dry deposition - ukca_sufddr
0	010	specific humidity after timestep	q	passed into chemistry routines
0	012	QCF	qcf	several places including ukca_sediment and calculation of ice optical depths for FastJ(X)
0	016	convective cloud liquid water path	conv_cloud_lwp	calculation of optical depths for FastJ(X)
0	024	surface temperature	tstar	used in dry deposition scheme
0	025	boundary layer depth	zbl	used in dry dep
0	026	roughness length	rough_length	used in old dry dep and for aerosol dep
0	030	land mask	land_sea_mask	used in emission_ctl
0	031	sea ice fraction	seaice_frac	used in dry dep
0	034	STANDARD DEVIATION OF OROGRAPHY	ho2r2_orog	used for dust scheme
0	058	SO2 surface emissions	part of all_emissions array	ukca_emission_ctl
0	060	ozone	um_ozone	top boundary condiiton
0	103	SO4 AITKEN MODE AEROSOL	so4_aitken	used in fastj(X)
0	104	SO4 AITKEN MODE AEROSOL	so4_accum	used in fastj(X)
0	121	SO2 volcanic emissions	so2_volc_3d	ukca_emission_ctl
0	126	High level SO2 Emissions	part of all_emissions array	ukca_emission_ctl
0	127	Ammonia emisisons	part of all_emissions array	ukca_emission_ctl
0	150	W COMPNT OF WIND	vertvel	used in ACTIVATE
0	211	CCA WITH ANVIL AFTER TIMESTEP	conv_cloud_amount	calculation of optical depths for FastJ(X)

Table 29: Prognostic driving fields used by UKCA – Continued

Sect	Item	Description	UKCA variable name	Where used
0	216	FRACTIONS OF SURFACE TYPES	frac_types	used in deposition and dust schemes
0	217	LEAF AREA INDEX OF PLANT FUNC TYPES	laift_lp	usedin dry dep
0	218	CANOPY HEIGHT OF PLANT FUNC TYPES	canectile_lp	usedin dry dep
0	229	CANOPY WATER ON TILES	canwctile_lp	usedin dry dep
0	233	SURFACE TEMPERATURE ON TILES	tstar_tile	Used in dry dep
0	234	ROUGHNESS LENGTH ON TILES	z0tile_lp	Used in dry dep
0	240	SNOW AMOUNT ON TILES	snow_tile	Used in dust scheme
0	253	DENSITY*R*R	rho_r2	Used in multiple places
0	254	QCL AFTER TIMESTEP	qcl	Fastj - odw calculation chemsitry dissolved fraction
0	255	EXNER PRESSURE (RHO)	exner_rho_levels	used in emission in call to trscrce
0	265	AREA CLOUD FRACTION IN EACH LAYER	area_cloud_fraction	Fastj odw calculation, chemistry dissolved fraction
0	266	BULK CLOUD FRACTION IN EACH LAYER	cloud_frac	passed to BE solver as zfcloud
0	267	LIQUID CLOUD FRACTION IN EACH LAYER	cloud_liq_frac	used in ACTIVATE and aerosol_ctl
0	301-320	Single level user ancil	part of all_emissions array	ukca_emission_ctl
0	322	Multi level user ancil	bc_biom_3d	ukca_emission_ctl
0	323	Multi level user ancil	oc_biom_3d	ukca_emission_ctl
0	324	Multi level user ancil	so2_biom_3d	ukca_emission_ctl
0	340	Multi level user ancil	aircraftems	ukca_emission_ctl
0	418	Dust parent soil clay fraction (anc)	soil_clay	Used in dust scheme
0	420	Dust parent soil sand fraction	soil_sand	Used in dust scheme
0	421	Dust soil mass fraction div 1	dust_mrel1	Used in dust scheme

Table 29: Prognostic driving fields used by UKCA – Continued

Sect	Item	Description	UKCA variable name	Where used
0	422	Dust soil mass fraction div 2	dust_mrel2	Used in dust scheme
0	423	Dust soil mass fraction div 3	dust_mrel3	Used in dust scheme
0	424	Dust soil mass fraction div 4	dust_mrel4	Used in dust scheme
0	425	Dust soil mass fraction div 5	dust_mrel5	Used in dust scheme
0	426	Dust soil mass fraction div 6	dust_mrel6	Used in dust scheme
0	505	Land fraction in grid box	fland	used in deposition and dust schemes and others
0	510	MEAN LAND ALBEDO AFTER TS	land_albedo	Set up to hold albedo for Fast-J (calculated from SW fluxes)

Table 30: Prognostic driving fields used by UKCA.

Sect	Item	Description	UKCA variable name	Where used
0	406	EXNER PRESSURE AT THETA LEVELS	exner_theta_levels	Yes - used to get t on theta levels in main
0	407	PRESSURE AT RHO LEVELS	p_rho_levels	used in main to get densities
0	408	PRESSURE AT THETA LEVELS	p_theta_levels	Yes - used to get t on theta levels in main
0	409	SURFACE PRESSURE	pstar	yes
1	201	NET DOWN SURFACE SW FLUX: SW TS ONLY	net_surf_sw	used to get albedo on radiation timesteps
1	235	TOTAL DOWNWARD SURFACE SW FLUX	tot_surf_sw	used to get albedo on radiation timesteps
2	284	SULPHATE OPTICAL DEPTH IN RADIATION	sulphate_od	used in fastjx
3	025	BOUNDARY LAYER DEPTH AFTER B.LAYER	ml_depth	used in call to tr_mix
3	060	RHOKH_MIX	rhokh_mix	used in call to tr_mix
3	064	DTRDZ_CHARNEY_GRID	dtrdz_charney_grid	used in call to tr_mix

Table 30: Diagnostic driving fields used by UKCA – Continued

Sect	Item	Description	UKCA variable name	Where used
3	065	GRID-LEVEL OF SML INVERSION (kent)	kent	used in call to tr_mix
3	066	Rho * entrainment rate (we_lim)	we_lim	used in call to tr_mix
3	067	Fraction of the timestep (t_frac)	t_frac	used in call to tr_mix
3	068	zrzi	zrzi	used in call to tr_mix
3	069	GRID-LEVEL OF DSC INVERSION	kent_dsc	used in call to tr_mix
3	070	Rho * entrainment rate dsc	we_lim_dsc	used in call to tr_mix
3	071	Fraction of the timestep dsc	t_frac_dsc	used in call to tr_mix
3	072	zrzi dsc	zrzi_dsc	used in call to tr_mix
3	073	ZHSC Top of decoupled layer	zhsc	used in call to tr_mix
3	217	SURFACE HEAT FLUX W/M2	surf_hf	used in dry dep
3	230	10 METRE WIND SPEED ON C-GRID	u_scalar_10m	used in aerosols to calculate sea-salt emissions
3	430	Dust Friction velocity (U*) on tiles	dust_ustar	used by dust scheme
3	462	STOMATAL CONDUCTANCE ON PFTS (M/S)	stcon	used by dry dep
3	465	FRICTION VELOCITY	u_s	used by dry dep
3	473	TURBULENT KINETIC ENERGY	bl_tke	used by ACTIVATE
4	205	CLOUD LIQUID WATER AFTER LS PRECIP	cloud_liq_water	used in activate and aerosol_ctl
4	222	RAINFALL RATE OUT OF MODEL LEVELS	ls_rain3d	used in chemistry and aerosols
4	223	SNOWFALL RATE OUT OF MODEL LEVELS	ls_snow3d	used in chemistry and aerosols
4	253	MELTING RATE OF ICE CRYSTALS	ice_melt	used for aerosol plume scavenging
4	254	MELTING RATE OF AGGREGATES	snow_melt	used for aerosol plume scavenging
4	257	RAIN AUTOCONVERSION RATE	autoconv	used for aerosol plume scavenging

Table 30: Diagnostic driving fields used by UKCA – Continued

Sect	Item	Description	UKCA variable name	Where used
4	258	RAIN ACCRETION RATE	accretion	used for aerosol plume scavenging
5	227	NOMINAL 3D CONVECTIVE RAINFALL RATE	conv_rain3d	used in chemistry and aerosols
5	228	NOMINAL 3D CONVECTIVE SNOWFALL RATE	conv_snow3d	used in chemistry and aerosols
5	218	LOWEST CONV CLOUD BASE LEVEL NO.	conv_cloud_base	used in FastJs to get optical depths lightning
5	219	LOWEST CONV CLOUD TOP LEVEL NO.	conv_cloud_top	used in FastJs to get optical depths lightning
8	242	CH4 FLUX FROM WETLAND KG C /M2/S	ch4_wetl_emiss	yes -emission
15	218	PV on model theta levels	pv_on_theta_mlevs	used in ukca_main to calculate tropopause pressure using a combined theta and PV surface
17	205	DMS emissions	part of all_emissions array	ukca_emission_ctl
30	453	Height at Tropopause Level	tropopause_height	Needed only for volcanic SO2 emissions into the stratosphere. (Always required as in call to emission_ctl)

Table 31: UKCA Fields optionally used in other sections.

Section	Item	Description	Usage
34	1	Ozone	Radiation and oxidant for CLASSIC
34	7	HNO3	CLASSIC nitrate aerosol code
34	8	H2O2	CLASSIC oxidant field
34	9	CH4	Radiation
34	49	N20	Radiation
34	55	CFC-11	Radiation (not to be used)
34	56	CFC-12	Radiation (not to be used)
34	81	OH	CLASSIC oxidant field (NR solver)

Section	Item	Description	Usage
34	82	HO2	CLASSIC oxidant field (NR solver)
34	103	ND_Ait_SOL	RADAER
34	104	Ait_SOL_SU	RADAER
34	105	Ait_SOL_BC	RADAER
34	106	Ait_SOL_BC	RADAER
34	107	ND_Acc_Sol	RADAER
34	108	Acc_SOL_SU	RADAER
34	109	Acc_SOL_BC	RADAER
34	110	Acc_SOL_OC	RADAER
34	111	Acc_SOL_SS	RADAER
34	113	ND_Cor_SOL	RADAER
34	114	Cor_SOL_SU	RADAER
34	115	Cor_SOL_BC	RADAER
34	116	Cor_SOL_OC	RADAER
34	117	Cor_SOL_SS	RADAER
34	118	Cor_SOL_DU	RADAER
34	119	ND_Ait_INS	RADAER
34	120	Ait_INS_BC	RADAER
34	121	Ait_INS_OC	RADAER
34	127	Ait_SOL_SS	RADAER
34	153	OH	CLASSIC oxidant field (BE solver)
34	154	HO2	CLASSIC oxidant field (BE solver)
34	162	CLOUD DROPLET NO. CONC.	Aerosol indirect effects
38	402	DRY PARTICLE DIAMETER AITKEN-SOL	RADAER
38	403	DRY PARTICLE DIAMETER ACCUMULATN-SOL	RADAER
38	404	DRY PARTICLE DIAMETER COARSE-SOL	RADAER
38	405	DRY PARTICLE DIAMETER AITKEN-INS	RADAER
38	409	WET PARTICLE DIAMETER AITKEN-SOL	RADAER
38	410	WET PARTICLE DIAMETER ACCUMULATN-SOL	RADAER
38	411	WET PARTICLE DIAMETER COARSE-SOL	RADAER
38	431	PTCL MASS DENSITY AITKEN-SOL (WET)	RADAER
38	432	PTCL MASS DENSITY ACCUM.-SOL (WET)	RADAER
38	433	PTCL MASS DENSITY COARSE-SOL (WET)	RADAER
38	434	PTCL MASS DENSITY AITKEN-INS	RADAER
38	446	SO4 PARTIAL VOLUME CONC (AIT-SOL)	RADAER
38	447	BC PARTIAL VOLUME CONC (AIT-SOL)	RADAER
38	448	OC1 PARTIAL VOLUME CONC (AIT-SOL)	RADAER
38	449	OC2 PARTIAL VOLUME CONC (AIT-SOL)	RADAER
38	450	H2O PARTIAL VOLUME CONC (AIT-SOL)	RADAER
38	451	SO4 PARTIAL VOLUME CONC (ACC-SOL)	RADAER
38	452	BC PARTIAL VOLUME CONC (ACC-SOL)	RADAER
38	453	OC1 PARTIAL VOLUME CONC (ACC-SOL)	RADAER

Section	Item	Description	Usage
38	454	SS PARTIAL VOLUME CONC (ACC-SOL)	RADAER
38	457	H2O PARTIAL VOLUME CONC (ACC-SOL)	RADAER
38	458	SO4 PARTIAL VOLUME CONC (COR-SOL)	RADAER
38	459	BC PARTIAL VOLUME CONC (COR-SOL)	RADAER
38	460	OC1 PARTIAL VOLUME CONC (COR-SOL)	RADAER
38	461	SSALT PARTIAL VOLUME CONC (COR-SOL)	RADAER
38	464	H2O PARTIAL VOLUME CONC (COR-SOL)	RADAER
38	465	BC PARTIAL VOLUME CONC (AIT-INS)	RADAER
38	466	OC1 PARTIAL VOLUME CONC (AIT-INS)	RADAER

C UKCA control variables set via rose edit

Table 32 indicates the logical control variables used for the chemistry scheme, table 33 indicates other setup variables used by UKCA.

Table 32: Logical control variables used by UKCA.

Variable	Feature
Chemistry Options	
L_UKCA	UKCA on
L_UKCA_CHEM_AERO	Use aerosol chemistry
L_UKCA_USE_2DTOP	Use 2-D top boundary files
L_UKCA_QCH4INTER	Interactive CH4 emissions
L_UKCA_INTDD	Interactive dry deposition scheme
L_UKCA_PRESCRIBECH4	Prescribe Surface CH4 MMRs
L_UKCA_SET_TRACE_GASES	Take UM trace gas MMR values (N2,H2) for LBCs/constant fields for ASAD in all chemistries
L_UKCA_HET_PSC	Heterogeneous/PSC chemistry
L_UKCA_TROPHET	Tropospheric heterogeneous chemistry
L_UKCA_SA_CLIM	Use aerosol climatology from SPARC in stratosphere, (with CLASSIC in troposphere)
L_UKCA_USE_BACKGROUND_AEROSOL	Use a single year (2100) value from climatology rather than 1950-2100
L_UKCA_RADO3	Use O3 in Radiation scheme
L_UKCA_RADCH4	Use CH4 in Radiation scheme
L_UKCA_H2O_FEEDBACK	Use H2O in Radiation scheme
L_UKCA_RADN2O	Use N2O in Radiation scheme
L_UKCA_RADF11	Use CFC-11 in Radiation scheme
L_UKCA_RADF12	Use CFC-12 in Radiation scheme
L_UKCA_RADF113	Use CFC-113 in Radiation scheme
L_UKCA_RADF22	Use HCFC-22 in Radiation scheme
L_UKCA_RADAER	Direct radiative effects of GLOMAP-mode aerosols
L_UKCA_RADAER_SUSTRAT	Use sulphuric acid optical properties for sulphate aerosol in the stratosphere
L_UKCA_AIE1	First aerosol indirect effect
L_UKCA_AIE2	Second aerosol indirect effect in activation scheme
MODE Options	
L_UKCA_MODE	Use MODE aerosol scheme

Table 32: Logical control variables used by UKCA – Continued

Variable	Feature
L_MODE_BHN_ON	Include binary nucleation
L_MODE_BLN_ON	Include boundary layer nucleation
L_UKCA_ARG_ACT	West activation scheme
L_UKCA_SFIX	Use fixed supersaturation value in West scheme
L_UKCA_PRIMSU	Primary SO4 emissions
L_UKCA_PRIMSS	Primary sea-salt emissions
L_UKCA_PRIMBCOC	Primary BC/OC emissions
L_BCOC_FF	Primary fossil fuel BC/OC emissions
L_BCOC_BF	Primary biofuel BC/OC emissions
L_BCOC_BM	Primary biomass BC/OC emissions

Table 33: Other setup variables

Variable	Type	Feature
Chemistry Options in UKCA namelist		
I_UKCA_CHEM	I	Chemistry scheme used
I_UKCA_PHOTOL	I	Photolysis scheme used
DTS0	I	B-E timestep
NIT	I	No. of B-E iterations
FASTJX_NUMWL	I	No. of wavelengths in Fastj-X (8, 12, or 18)
FASTJX_PRESCUTOFF	R	Prescribed cutoff pressure (hPa)
FASTJX_MODE	R	2D, merge or Fastj-X above cutoff
JVSPEC_DIR	C	Directory for spectral files
JVSPEC_FILE	C	Spectral (X-section) file name
JVSCAT_FILE	C	Scattering file name
PHOT2D_DIR	C	Directory for 2D photolysis file
STRAT2D_DIR	C	Directory for 2D upper boundary data
DIR_STRAT_AER	C	Directory for stratospheric aerosol file
FILE_STRAT_AER	C	File for stratospheric aerosol data
I_UKCA_SCENARIO	I	Takes trace gas MMR values from the values in the run_radiation namelist(=0), the WMOA1 scenario (=1), or from a file (=2) located at UKCA_RCPDIR/UKCA_RCPFILE, for Lower BCs in Strat/CheST
UKCA_MeBrMMR	R	MeBr trace-gas MMR
UKCA_MeClMMR	R	MeCl trace-gas MMR

Table 33: Other setup variables used by UKCA (continued)

Variable	Type	Feature
UKCA_CH2Br2MMR	R	CH2Br2 trace-gas MMR
UKCA_CFC115MMR	R	CFC115 trace-gas MMR
UKCA_CCl4MMR	R	CCl4 trace-gas MMR
UKCA_MeCCl3MMR	R	MeCCl3 trace-gas MMR
UKCA_HCFC141bMMR	R	HCFC141b trace-gas MMR
UKCA_HCFC142bMMR	R	HCFC142b trace-gas MMR
UKCA_H1211MMR	R	H1211 trace-gas MMR
UKCA_H1202MMR	R	H1202 trace-gas MMR
UKCA_H1301MMR	R	H1301 trace-gas MMR
UKCA_H2402MMR	R	H2402 trace-gas MMR
UKCA_COSMMR	R	COS trace-gas MMR
UKCA_H2MMR	R	H2 trace-gas MMR
UKCA_N2MMR	R	N2 trace-gas MMR
UKCA_RCPDIR	C	Directory containing RCP file
UKCA_RCPFILE	C	Name of RCP file
Aerosol Options in UKCA namelist		
I_MODE_SETUP	I	Defines MODE aerosol scheme
I_MODE_BLN_PARAM_METHOD	I	Defines BLN parametrisation
I_MODE_NZTS	I	No. substeps for nucl/sedimentation
MODE_PARFRAC	R	Fraction of SO2 emission as aerosol
MODE_AITSOL_CVSCAV	R	Fraction of Aitken mode affected by plume scavenging
Options in NLSCATM namelist		
L_UKCA	L	UKCA on
L_UKCA_RADAER	L	Direct radiative effects of GLOMAP-mode aerosols
L_UKCA_RADAER_SUSTRAT	L	Use sulphuric acid optical properties for sulphate aerosol in the stratosphere
L_UKCA_AIE1	L	First aerosol indirect effect
L_UKCA_AIE1 IS NOT OPERATIONAL		
L_UKCA_AIE2	L	Second aerosol indirect effect in activation scheme
L_UKCA_AIE2 IS NOT OPERATIONAL		
UKCA_INT_METHOD	I	Defines chemical integration method

Table 34: Control variables set in the code.

Variable	Feature	State	Routine
Chemistry Options			
L_USE_UMO3	Use UM ozone field for upper BC	TRUE	ukca_stratf
L_USE_O3HNO3ratio	Used fixed O3:HNO3 ratio for upper BC	TRUE	ukca_stratf
L_ALL_STRAT	Overwrite stratospheric concentrations a fixed number of levels above tropopause	TRUE	ukca_stratf
L_OVERWRITE_CH4	Overwrite CH4 with 2D boundary conditions	FALSE	ukca_stratf
L_UKCA_DIURNAL_ISOPEMS	Call routine to give diurnal cycle to isoprene emissions	TRUE	ukca_emission_ctl
L_USE_STRATCLIM	Add stratospheric aerosol climatology optical depth calculation	FALSE	ukca_fastjx
L_UKCA_TEST_SCENARIO_RCP	Call the routine TEST_SCENARIO_RCP_CTL from the UKCA_SCENARIO_CTL routine to test the output produced by UKCA_SCENARIO_RCP	FALSE	ukca_scenario_rcp_mod
Aerosol Options			
I_BHN_METHOD	Binary homogeneous nucleation method	2	UKCA_CALCNUCRATE
I_NUC_METHOD	How B/L nucleation is applied	2	UKCA_AERO_CTL
I_MODE_NUCSCAV	Defines nucleation scavenging	1	UKCA_OPTION_MOD
I_MODE_SS_SCHEME	Defines sea-salt emission scheme	1	UKCA_OPTION_MOD
L_UKCA_PLUME_SCAV	Use convective plume scavenging	TRUE	UKCA_OPTION_MOD

D UKCA Standard Diagnostics

Table 35: UKCA Standard Diagnostics provided by the ASAD diagnostics package. NOTE: Any O_x budget is in mole of O_x/ gridcell/second. All other diagnostics are in mole/gridcell/second unless otherwise stated.

STASH code	Scheme(s)	Description
50001	TropIsop, CheST	O_x Production: NO + HO_2
50002	TropIsop, CheST	O_x Production: NO + CH_3OO
50003	TropIsop, CheST	O_x Production: NO + RO_2
50004	TropIsop, CheST	O_x Production: OH + Inorganic Acid
50005	TropIsop, CheST	O_x Production: OH + Organic Nitrate
50006	TropIsop, CheST	O_x Production: Organic Nitrate Photolysis
50007	TropIsop, CheST	O_x Production: OH + PAN-type Reactions
50011	TropIsop, CheST	O_x Loss: $O(^1D)$ + H_2O
50012	TropIsop, CheST	O_x Loss: Minor Reactions
50013	TropIsop, CheST	O_x Loss: O_3 + HO_2
50014	TropIsop, CheST	O_x Loss: O_3 + OH
50015	TropIsop, CheST	O_x Loss: O_3 + Alkene
50016	TropIsop, CheST	O_x Loss: N_2O_5 + H_2O
50017	TropIsop, CheST	O_x Loss: NO_3 Chemical Loss
50021	TropIsop, CheST	O_x Dry Deposition: O_3 Dry Deposition
50022	TropIsop, CheST	O_x Dry Deposition: NO_y Dry Deposition
50031	TropIsop, CheST	O_x Wet Deposition: NO_y Wet Deposition
50041	All	Tropospheric CH_4 Lifetime
50042	TropIsop, CheST	NO_3 + C_5H_8
50043	TropIsop, CheST	NO + ISO2
50044	TropIsop, CheST	HO_2 + HO_2
50045	TropIsop, CheST	HO_2 + RO_2
50046	TropIsop, CheST	HO_2 + NO_2
50051	All	O_3 STE
50052	All	Tropospheric O_3 Tendency
50053	All	Tropospheric O_3 MMR
50054	All	O_3 Tendency
50061	All	Tropospheric Mass of Air
50062	All	Tropospheric Mask (fraction)
50063	All	Mass of Air
50071	TropIsop, CheST	CO Loss: CO + OH
50072	TropIsop, CheST	CO Production: HCHO + OH/NO_3
50073	TropIsop, CheST	CO Production: MGLY + OH/NO_3
50074	TropIsop, CheST	CO Production: O_3 + MACR/C_5H_8 & other fluxes
50075	TropIsop, CheST	CO Production: HCHO Photolysis (Radical)

Table 35: UKCA Standard Diagnostics (continued)

STASH code	Scheme(s)	Description
50076	TropIsop, CheST	CO Production: HCHO Photolysis (Molecular)
50077	TropIsop, CheST	CO Production: MGLY Photolysis
50078	TropIsop, CheST	CO Production: Other CO Photolysis Reactions
50079	TropIsop, CheST	CO Dry Deposition
50081	All	Lightning Diagnostics: NOx Emissions
50082	All	Lightning Diagnostics: Total Flash Rate in flashes/gridcell/min (2D)
50083	All	Lightning Diagnostics: Cloud-to-Ground Flash Rate in flashes/gridcell/min (2D)
50084	All	Lightning Diagnostics: Cloud-to-Cloud Flash Rate in flashes/gridcell/min (2D)
50085	All	Lightning Diagnostics: N Produced kg(N)/m^2/s (2D)
50091	Strat, CheST	Stratospheric OH Production
50092	Strat, CheST	Stratospheric OH Loss
50101	Strat	Stratospheric O_x Production: O_2 Photolysis
50102	Strat	Stratospheric O_x Production: HO_2 + NO
50103	Strat	Stratospheric O_x Production: CH_3OO + NO
50104	Strat	Stratospheric O_x Production: OH + HNO_3
50111	Strat	Stratospheric O_x Loss: Cl_2O_2 Photolysis
50112	Strat	Stratospheric O_x Loss: BrO + ClO
50113	Strat	Stratospheric O_x Loss: HO_2 + O_3
50114	Strat	Stratospheric O_x Loss: HO_2 + ClO
50115	Strat	Stratospheric O_x Loss: HO_2 + BrO
50116	Strat	Stratospheric O_x Loss: $O(^3P)$ + ClO
50117	Strat	Stratospheric O_x Loss: $O(^3P)$ + NO_2
50118	Strat	Stratospheric O_x Loss: $O(^3P)$ + HO_2
50119	Strat	Stratospheric O_x Loss: O_3 + H
50120	Strat	Stratospheric O_x Loss: O_3 + $O(^3P)$
50121	Strat	Stratospheric O_x Loss: NO_3 Photolysis
50122	Strat	Stratospheric O_x Loss: $O(^1D)$ + H_2O
50123	Strat	Stratospheric O_x Loss: NO_3 + HO_2
50124	Strat	Stratospheric O_x Loss: NO_3 + OH
50125	Strat	Stratospheric O_x Loss: NO_3 + HCHO
50131	CheST, Strat	O_x Deposition: O_3 Dry Deposition
50132	CheST, Strat	O_x Deposition: NO_y Dry Deposition
50133	CheST, Strat	O_x Deposition: NO_y Wet Deposition
50140	Strat, Strattrop and	DMS + OH → SO_2 + CH_3OO + HCHO
50141	Tropisop Aerosol	DMS + OH → SO_2 + CH_3OO + DMSO
50142	——- ” ———-	DMS + NO_3
50143	——- ” ———-	OH + DMSO

Table 35: UKCA Standard Diagnostics (continued)

STASH code	Scheme(s)	Description
50144	——- ” ———-	OH + CS_2
50145	——- ” ———-	OH + H_2S
50146	——- ” ———-	OH + COS
50150	——- ” ———-	SO_2 + OH
50151	——- ” ———-	HSO_3^- + H_2O_2 (aq) equivalent reaction
50152	——- ” ———-	HSO_3^- + O_3 (aq) equivalent reaction
50153	——- ” ———-	$SO_3^- -$ + O_3 (aq) equivalent reaction
50154	——- ” ———-	SO_2 Dry Deposition
50155	——- ” ———-	SO_2 Wet Deposition
50147	Strattrop and Tropisop	Monoterpene + OH
50148	Aerosol schemes	Monoterpene + O_3
50149	——- ” ———-	Monoterpene + NO_3

Note that when using the CHEST (aka Strat-trop) scheme, two different STASHcodes are available for 3 diagnostics. O_3 Dry Deposition can be output either as 50.021 or 50.131; Dry Deposition: NO_y Dry Deposition as 50.022 or 50.132; NO_y Wet Deposition as 50.031 or or 50.133. These should be equivalent.

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