Treatment of emissions in UKCA

Introduction to UKCA, 5-9 Jan 2015, Cambridge

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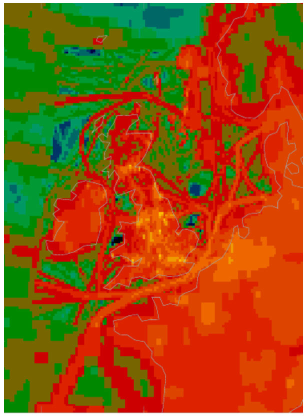
Treatment of emissions in UKCA

1. Introduction
2. Ancillary emission system
3. NetCDF emission system
4. Final notes

1. Introduction

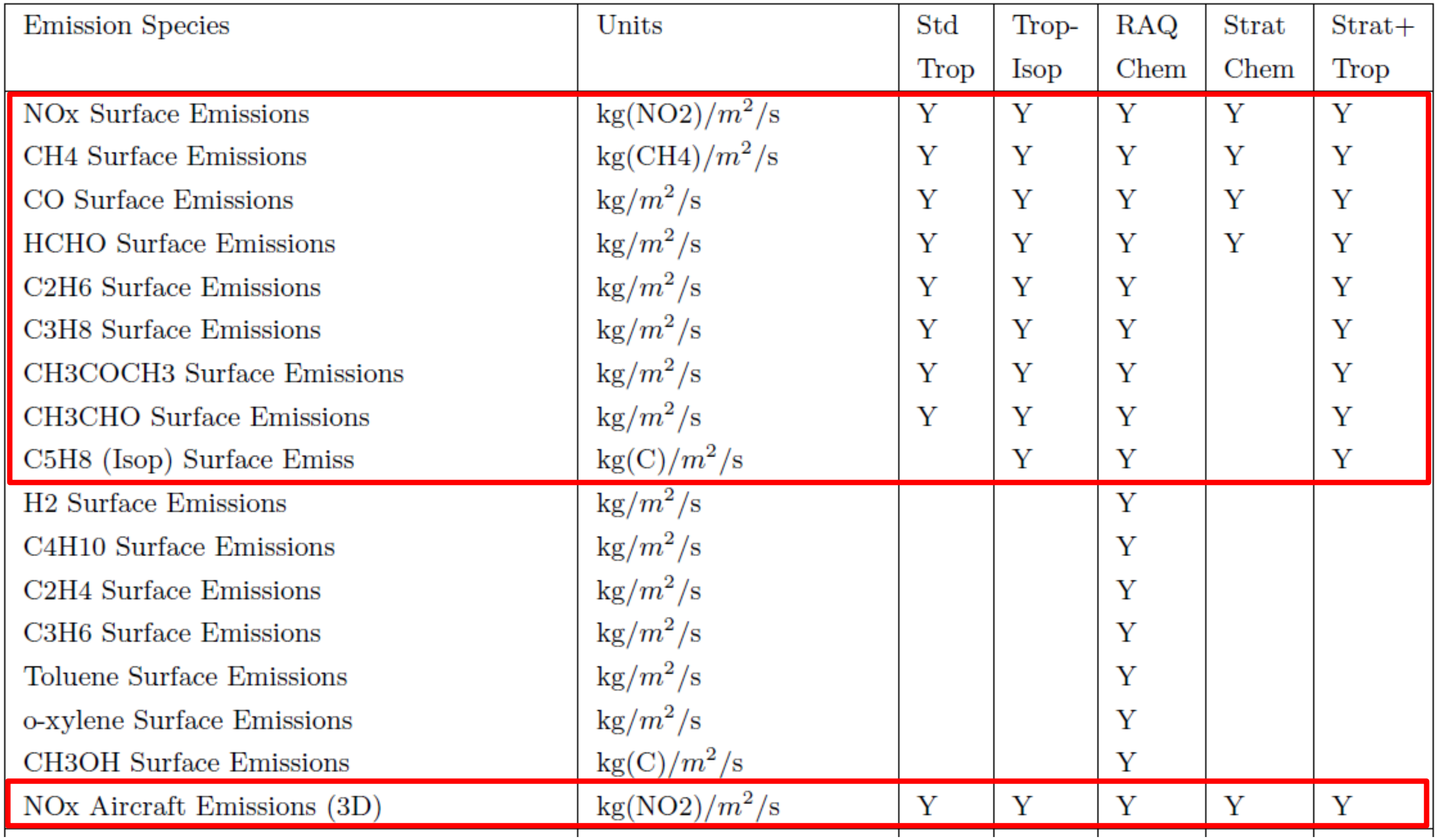
Emission inputs to UKCA

- Offline: Pre-computed fluxes
  - Read in from ancillary or NetCDF files
  - 12-monthly varying 2-D or 3-D fields



- Online: Computed in real-time using fields from the UM. Examples:
  - Lightning NO_x
  - Sea-salt (in GLOMAP-mode)
  - Wetland CH_4 (from JULES)
  - Interactive BVOC (from JULES; for isoprene, terpenes, methanol, acetone; since UM vn9.2).

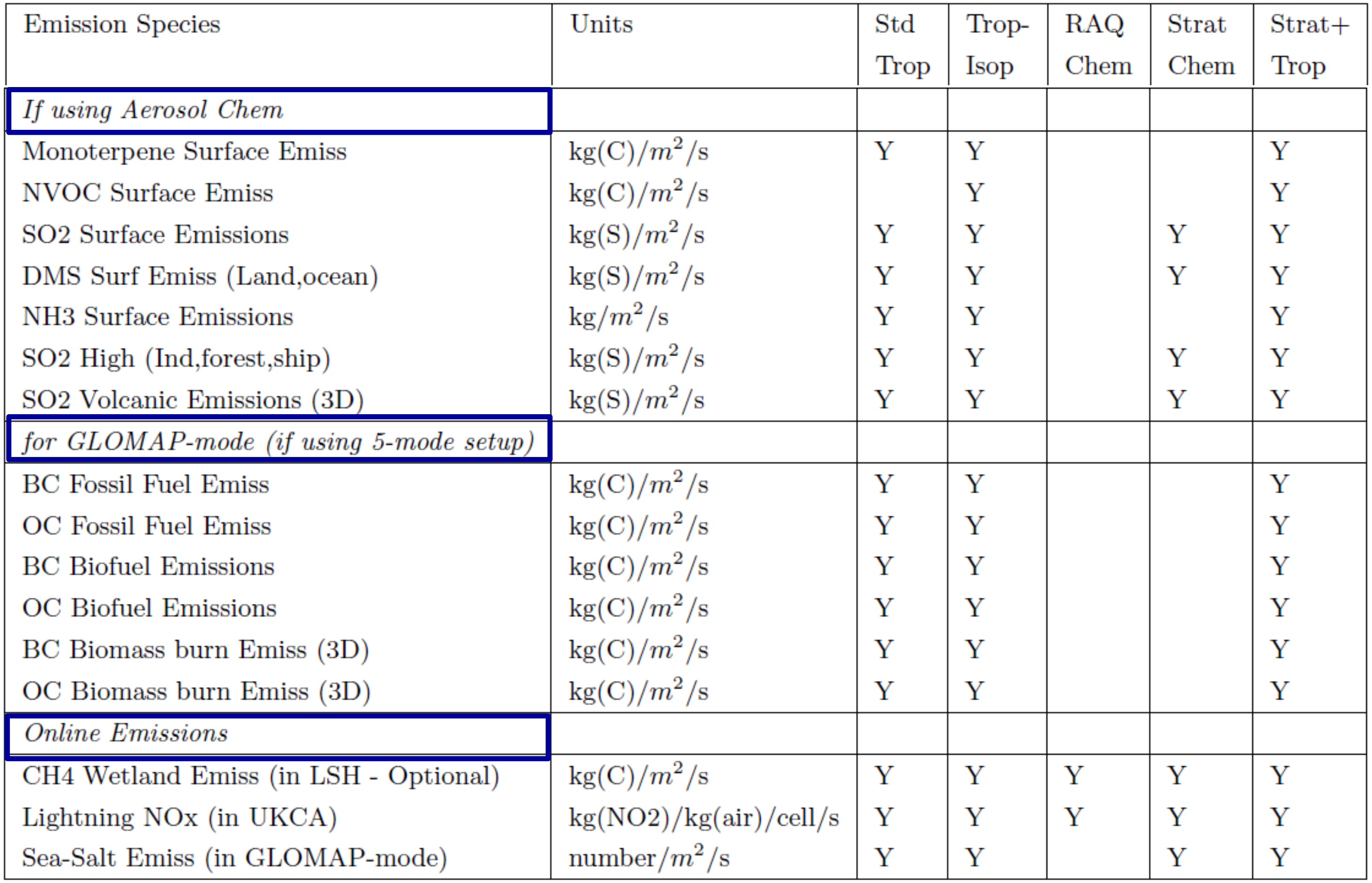
Gas phase emissions



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

(Taken from UMDP 084 for UKCA)

Aerosol & online emissions



Emission Species	Units	Std Trop	Trop-Isop	RAQ Chem	Strat Chem	Strat+Trop
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

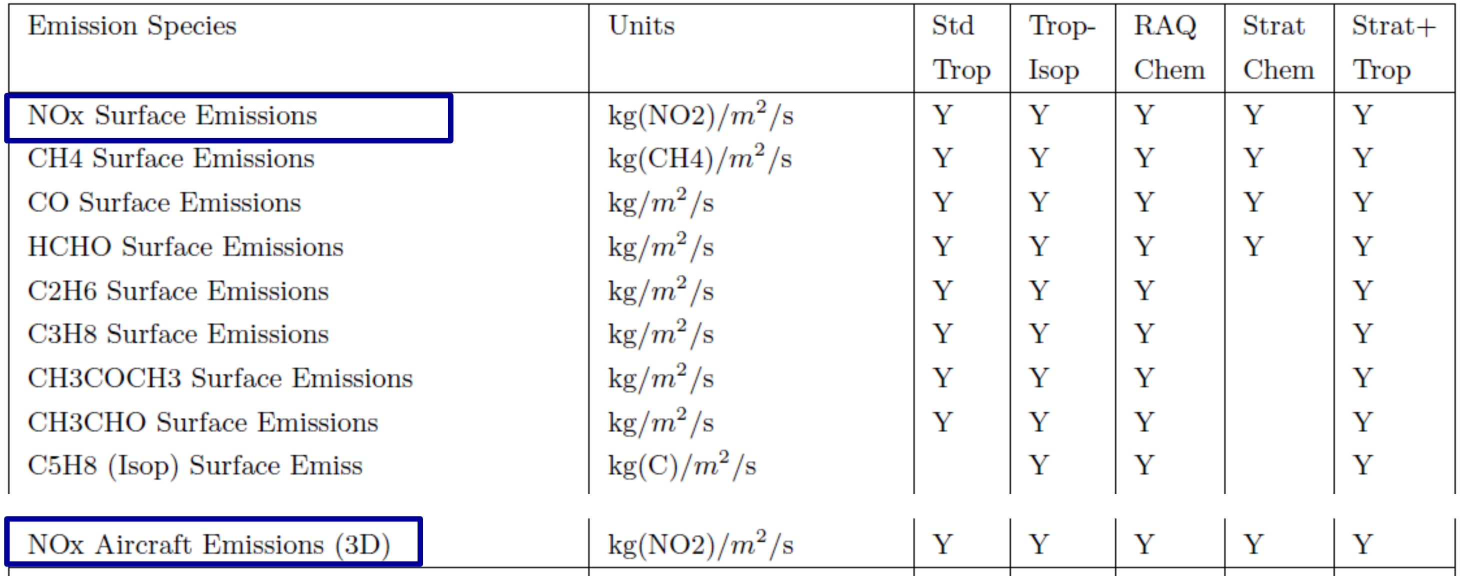
(Taken from UMDP 084 for UKCA)

2. Ancillary emission system

Emission files & STASH

UKCA Makes use of user ancillary files:

- single-level: items 301-320 (STASH section 0)
- multi-level: items 321-340 (STASH section 0)



STASH code	Emission Species	Units	Std Trop	Trop-Isop	RAQ Chem	Strat Chem	Strat+Trop
301	NOx Surface Emissions	kg(NO2)/m^2/s	Y	Y	Y	Y	Y
302	CH4 Surface Emissions	kg(CH4)/m^2/s	Y	Y	Y	Y	Y
303	CO Surface Emissions	kg/m^2/s	Y	Y	Y	Y	Y
304	HCHO Surface Emissions	kg/m^2/s	Y	Y	Y	Y	Y
305	C2H6 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
306	C3H8 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
307	CH3COCH3 Surface Emissions	kg/m^2/s	Y	Y	Y		Y
308	CH3CHO Surface Emissions	kg/m^2/s	Y	Y	Y		Y
309	C5H8 (Isop) Surface Emiss	kg(C)/m^2/s		Y	Y		Y
...							
340	NOx Aircraft Emissions (3D)	kg(NO2)/m^2/s	Y	Y	Y	Y	Y

Rest of items in section 0 reserved for UM prognostics

Need to add STASH items

LevelT | LevelF | LevelL

```
#
1|     1 |     0 |   301 |NOx surf emissions                 |
2|     2 |     0 |     1 |     1 |     5 |    -1 |    -1 |     0 |     0 |     0 |     0 |
3| 000000000000000000000000000000 | 00000000000000000001 |     3 |
4|     1 |     0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
5|     0 |   531 |     0 |   129 |     0 |     0 |     0 |     0 |     0 |
#
```

LBVC

```
#
1|     1 |     0 |   340 |NOX AIRCRAFT EMS IN KG/S/GRIDCELL    |
2|     2 |     0 |     1 |     1 |     2 |    10 |    11 |     0 |     0 |     0 |     0 |
3| 000000000000000000000000000000 | 00000000000000000001 |     3 |
4|     1 |     0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
5|     0 |   520 |    20 |    65 |     0 |     0 |     0 |  9999 |     0 |
#
```

Meaning:

- Item 301: Single level data (surface level)
- Item 340: Data on atmosphere theta levels (from first to last tracer level)

More info in UMDP C4 “Storage Handling And Diagnostic System (STASH)”

Basically 2-D fields will be like 301 and 3-D like 340.

Array “em_chem_spec” (1)

- **Array with list of emitted species/fields**
  Scheme specific. Declared in **ukca_d1_defs.F90**:
  `CHARACTER(LEN=10), DIMENSION(:), ALLOCATABLE, SAVE :: em_chem_spec`

- **Allocated & filled in ukca_setd1defs.F90**

(IF block for different chemistry schemes)

```
...
ELSE IF (L_UKCA_RAQ) THEN      ! Regional air quality chemistry (RAQ)
   n_chem_emissions  = 16
   n_3d_emissions    = 1       ! aircraft NOx
   ALLOCATE(em_chem_spec(n_chem_emissions+n_3d_emissions))
   em_chem_spec =                                                &
     (/'NO        ','CH4       ','CO        ','HCHO      ',      &
       'C2H6      ','C3H8      ','Me2CO     ','MeCHO     ',      &
       'C5H8      ','C4H10     ','C2H4      ','C3H6      ',      &
       ‘TOLUENE   ','oXYLENE   ','CH3OH     ','H2        ',      &
       'NO_aircrft' /)
```

NO$_x$ emissions: Expressed as kg(NO$_2$) m^{-2} s^{-1} but assigned to the NO tracer!

Array “em_chem_spec” (2)

```
...
 ELSE IF (L_ukca_strattrop .AND. L_ukca_achem) THEN
     n_chem_emissions = 21
     n_3d_emissions   = 2       ! volc SO2 & aircraft NOX
     ALLOCATE(em_chem_spec(n_chem_emissions+n_3d_emissions))
     em_chem_spec =                                           &
       (/'NO        ','CH4       ','CO        ','HCHO      ', &
         'C2H6      ','C3H8      ','Me2CO     ','MeCHO     ', &
         'C5H8      ','BC_fossil ','BC_biofuel','OC_fossil ', &
         'OC_biofuel','Monoterp  ','NVOC      ','SO2_low   ', &
         'SO2_high  ','NH3       ','DMS       ','SO2_nat   ', &
         'BC_biomass','OC_biomass','NO_aircrft'/)
```

NO_x emissions: Expressed as kg(NO_2) m^{-2} s^{-1} but assigned to the NO tracer!

If adding new emission field:

- Look for your chemistry scheme in the IF block of UKCA_SETD1DEFS. Update em_chem_spec.
- Need new STASH code?
- Need to update long block towards the end of UKCA_SETD1DEFS?

(See tutorial in the afternoon)

Code in UKCA_MAIN
(ukca_main1-ukca_main1.F90)

```
IF ( L_ukca_new_emiss )  THEN
         CALL ukca_new_emiss_ctl ( ... )
ELSE
         CALL UKCA_EMISSION_CTL  ( ... )
END IF
```

NetCDF (since UM vn8.6)

ancillaries

Both cases accept online emissions

ukca_emission_ctl.F90 (1)

Beginning of the routine ➔ Some initialisations & IF blocks affecting different UKCA configurations/options. Examples:

```
! Call routine for primary emissions for UKCA-MODE
IF (L_ukca_mode) THEN                 ! Number & mass emission fluxes
    CALL ukca_mode_ems_um             ! are assembled for each tracer
END IF                                ! in array em_field_mode


! Regrid interative BVOC emissions from landpoints (1D) to 2D-grid
IF (L_bvoc_emis) THEN
  We get isoprene_2D, terpene_2D, methanol_2D, acetone_2D
END IF
```

Then very **long loop through all gas phase tracers** to (i) **add surface emissions**, including unit conversions if needed, and (ii) do **boundary layer mixing of tracers**. See next slide …

ukca_emission_ctl.F90 (2)

```
!   Check if tracer has surface emissions and set emission. Otherwise emission field is zero from initialisation.
DO k = 1, jpctr            ! loop over tracers
    DO l = 1, n_chem_emissions








!       Rest of emissions
        ELSE IF (advt(k) == em_chem_spec(l) ) THEN
          em_field(:,:,k) = all_emissions(:,:,l)
        ENDIF            ! end advt(k)
   END DO     !  l=1,n_use_emissions








END DO       ! end of loop over tracers
```

ukca_emission_ctl.F90 (2)

```
!   Check if tracer has surface emissions and set emission. Otherwise emission field is zero from initialisation.
DO k = 1, jpctr              ! loop over tracers
    DO l = 1, n_chem_emissions
        IF (advt(k) == em_chem_spec(l) .AND. em_chem_spec(l) == 'NO      ' ) THEN
!            Convert from kg NO2/m2/s to kg NO/m2/s
             em_field (:,:,k) = all_emissions (:,:,l) * m_no / m_no2







!        Rest of emissions
        ELSE IF (advt(k) == em_chem_spec(l) ) THEN
             em_field(:,:,k) = all_emissions(:,:,l)
        ENDIF              ! end advt(k)
    END DO      !  l=1,n_use_emissions








END DO       ! end of loop over tracers
```

ukca_emission_ctl.F90 (2)

```
!   Check if tracer has surface emissions and set emission. Otherwise emission field is zero from initialisation.
DO k = 1, jpctr             ! loop over tracers
   DO l = 1, n_chem_emissions
      IF (advt(k) == em_chem_spec(l) .AND. em_chem_spec(l) == 'NO      ' ) THEN
!         Convert from kg NO2/m2/s to kg NO/m2/s
          em_field (:,:,k) = all_emissions (:,:,l) * m_no / m_no2

      ELSE IF …      !  Many other checks  (for SO2_low, DMS, Monoterp, C5H8,  MeOH, Me2CO, ...).
!                       Note that BVOC emissions might be interactive
!
!         If you update the code check if there are specific unit conversions for your
!         species and make sure that is consistent with your emission fields.
        ….

!        Rest of emissions
      ELSE IF (advt(k) == em_chem_spec(l) ) THEN
          em_field(:,:,k) = all_emissions(:,:,l)
      ENDIF          ! end advt(k)
   END DO      !  l=1,n_use_emissions




END DO      ! end of loop over tracers
```

ukca_emission_ctl.F90 (2)

```
!   Check if tracer has surface emissions and set emission. Otherwise emission field is zero from initialisation.
DO k = 1, jpctr              ! loop over tracers
    DO l = 1, n_chem_emissions
        IF (advt(k) == em_chem_spec(l) .AND. em_chem_spec(l) == 'NO      ' ) THEN
!         Convert from kg NO2/m2/s to kg NO/m2/s
          em_field (:,:,k) = all_emissions (:,:,l) * m_no / m_no2

        ELSE IF …      !  Many other checks  (for SO2_low, DMS, Monoterp, C5H8,  MeOH, Me2CO, ...).
!                         Note that BVOC emissions might be interactive
!
!       If you update the code check if there are specific unit conversions for your
!       species and make sure that is consistent with your emission fields.
      ….

!       Rest of emissions
        ELSE IF (advt(k) == em_chem_spec(l) ) THEN
          em_field(:,:,k) = all_emissions(:,:,l)
        ENDIF          ! end advt(k)
    END DO      !  l=1,n_use_emissions

    IF (advt(k) == 'CH4      '  … ) THEN
!       Add wetland CH4 emissions or prescribe the surface mixing ratio

    IF (L_ukca_strat .OR. L_ukca_stratcfc .OR.  L_ukca_strattrop)  THEN
 !      Treatment of long-lived species with lower boundary condition



END DO        ! end of loop over tracers
```

Met Office

ukca_emission_ctl.F90 (2)

```
!   Check if tracer has surface emissions and set emission. Otherwise emission field is zero from initialisation.
DO k = 1, jpctr              ! loop over tracers
    DO l = 1, n_chem_emissions
        IF (advt(k) == em_chem_spec(l) .AND. em_chem_spec(l) == 'NO      ' ) THEN
!           Convert from kg NO2/m2/s to kg NO/m2/s
           em_field (:,:,k) = all_emissions (:,:,l) * m_no / m_no2

        ELSE IF …      !  Many other checks  (for SO2_low, DMS, Monoterp, C5H8,  MeOH, Me2CO, ...).
!                         Note that BVOC emissions might be interactive
!
!       If you update the code check if there are specific unit conversions for your
!       species and make sure that is consistent with your emission fields.
      ….

!       Rest of emissions
        ELSE IF (advt(k) == em_chem_spec(l) ) THEN
           em_field(:,:,k) = all_emissions(:,:,l)
        ENDIF          ! end advt(k)
    END DO      !  l=1,n_use_emissions

    IF (advt(k) == 'CH4      '  … ) THEN
!       Add wetland CH4 emissions or prescribe the surface mixing ratio

    IF (L_ukca_strat .OR. L_ukca_stratcfc .OR.  L_ukca_strattrop)  THEN
 !       Treatment of long-lived species with lower boundary condition

!   Call boundary layer mixing and add surface emissions.
        CALL TR_MIX ( …,  em_field (:, :, k), … , tracers (:, :, 1:bl_levels, k), ….)

END DO        ! end of loop over tracers
```

ukca_emission_ctl.F90 (3a)

Similar stuff for GLOMAP-mode

```
! Beginning of ukca_emission_ctl. Call routine for primary emissions for UKCA-MODE
        IF (L_ukca_mode) THEN
            CALL ukca_mode_ems_um    ➔ em_field_mode is filled with nr & mass
        END IF                           emission fluxes for each tracer
```

1. Initial emission arrays for aerosols are created from the **input data** (depending on the model set-up)

2. **CALL ukca_mode_ems:** returns **mass** & **number emission arrays** for sulphate, sea-salt, OC, BC and dust (as required)

3. The number and mass fluxes are then assembled for each tracer in the **array em_field_mode**

4. **Diagnostics** for emitted component mass are stored in STASH

38	201	PRIMARY SO4 TO AITKEN (SOL)
38	202	PRIMARY SO4 TO ACCUMULATION (SOL)
38	203	PRIMARY SO4 TO COARSE (SOL)
38	204	PRIMARY SEA-SALT TO ACCUMULTN (SOL)
38	205	PRIMARY SEA-SALT TO COARSE (SOL)
38	206	PRIMARY BLACK CARBON TO AITKEN (SOL)
38	207	PRIMARY BLACK CARBON TO AITKEN (INS)
38	208	PRIMARY ORG. CARBON TO AITKEN (SOL)
38	209	PRIMARY ORG. CARBON TO AITKEN (INS)
38	210	PRIMARY DUST TO ACCUMULATION (SOL)
38	211	PRIMARY DUST TO ACCUMULATION (INS)
38	212	PRIMARY DUST TO COARSE (SOLUBLE)

ukca_emission_ctl.F90 (3b)

Similar stuff for GLOMAP-mode

```
! Beginning of ukca_emission_ctl. Call routine for primary emissions for UKCA-MODE
        IF (L_ukca_mode) THEN
            CALL ukca_mode_ems_um   ➔  em_field_mode is filled with nr & mass
        END IF                         emission fluxes for each tracer


! After doing injection & mixing of gas tracers. Do same for MODE aerosols

        IF (L_ukca_mode) THEN

          ! Call boundary layer mixing and add surface emissions
          ! for GLOMAP-mode aerosol tracers

          DO kaer = 1,n_mode_tracers                ! loop over tracers

             CALL TR_MIX (..., em_field_mode (:, :, 1,           kaer), ...,
                               mode_tracers  (:, :, 1:bl_levels, kaer), ...)




          END DO                           ! end of loop over tracers (kaer)

        END IF ! if L_UKCA_MODE
```

ukca_emission_ctl.F90 (3b)

Similar stuff for GLOMAP-mode

```
! Beginning of ukca_emission_ctl. Call routine for primary emissions for UKCA-MODE
        IF (L_ukca_mode) THEN
            CALL ukca_mode_ems_um    ➔ em_field_mode is filled with nr & mass
        END IF                         emission fluxes for each tracer


! After doing injection & mixing of gas tracers. Do same for MODE aerosols

        IF (L_ukca_mode) THEN

          ! Call boundary layer mixing and add surface emissions
          ! for GLOMAP-mode aerosol tracers

          DO kaer = 1,n_mode_tracers                 ! loop over tracers

           CALL TR_MIX (...,  em_field_mode (:, :, 1,            kaer), ...,
                              mode_tracers  (:, :, 1:bl_levels, kaer), ...)


            ! Add in emission fluxes not at surface level
            DO k = 2,model_levels
               CALL TRSRCE (..., mode_tracers (:, :, k, kaer), ...,
                                 em_field_mode(:, :, k, kaer), ...)
            END DO ! loop over model levels 2 to top (k)


          END DO                           ! end of loop over tracers (kaer)

        END IF ! if L_UKCA_MODE
```

ukca_emission_ctl.F90 (4)

```
! Diagnose NO2 lightning emissions
  lightningem_n_gridbox   = 0.0
  lightningem_no2_to_air = 0.0
  CALL UKCA_LIGHT_CTL( ...                                           &
     lightningem_n_gridbox  (1:row_length,1:rows,1:model_levels),   &
     lightningem_no2_to_air (1:row_length,1:rows,1:model_levels))
```

```
! Convert aircraft emissions from kg NO2/gridbox/s to kg NO/m2/s
 Within some loops:
    conv_aircraftems(j,k,l)   = aircraftems(j,k,l)                  &
      * m_no/(surf_area(j,k)*m_no2)

! Add aircraft emissions to NO or NOx tracer
  DO k = 1,model_levels
    CALL TRSRCE (                                                    &
       ..., tracers(:,:,k,inox), conv_aircraftems(:,:,k), k, …)
  END DO
```

```
! Update tracer fields with NO/NOx lightning emissions
     tracers(1:row_length,1:rows,:,inox) =                           &
          tracers(1:row_length,1:rows,:,inox) +                     &
          timestep*lightningem_no2_to_air*m_no/m_no2
```

ukca_emission_ctl.F90 (5)

Finally, **treatment of SO_2 emissions** (if aerosol chemistry):

- Add (3-D volcanic + high-level anthropogenic) emissions to SO_2 tracer.

  NOTE: The code removes direct sulphate fraction of emissions and converts from kg(S) to kg (SO_2)

- Add 3-D emissions from explosive volcanic eruptions (e.g. Pinatubo 1991 and 5 others):

```
CALL UKCA_VOLCANIC_SO2
```

Last note (only for ASAD framework). Some calls to output emission diagnostics:

```
CALL asad_emissions_diagnostics
CALL asad_3D_emissions_diagnostics
```

Advantages and limitations of the ancillary emission system

Advantages

Well tested for all UKCA configurations:

- Works with all chemistry schemes & with GLOMAP-mode
- UKCA_EMISSION_CTL accepts all online emissions available in UKCA

Limitations

- Cannot easily treat emissions from independent source sectors separately. Example:

```
em_chem_spec =                                   &
  (/'NO        ',....                            &
    'SO2_low   ', 'SO2_high  `, 'SO2_nat   ',    &
    ..., 'NO_aircrft'/)
```

- Units in emission fields need to be as indicated in UKCA_EMISSION_CTL. However the UKCA code cannot check whether that is the case in your ancillary emission file!

3. NetCDF emission system

Introduction

Available since UM vn8.6

Advantages

- Allow the use of different emission fields to account for independent source sectors for any given tracer
- Emissions can be injected at different altitudes and with different temporal variability
- Avoid inconsistencies in the units of the emission fields (to comply with CF conventions units should be “kg m^{-2} s^{-1}”)

Limitations

- Currently tested only for RAQ & Strat-Trop chemistry
- Needs to be extended for:
  - aerosol emissions (l_ukca_mode .OR. l_ukca_aerchem .OR. l_ukca_nr_aqchem)
  - iBVOC emissions (L_ukca_ibvoc .AND. L_bvoc_emis)

UKCA code for NetCDF emissions

- As before “**em_chem_spec**” is allocated & filled within **ukca_setd1defs.F90**

  Each element of the array could correspond to 1 or more emission fields

- From **ukca_main1-ukca_main1.F90**:

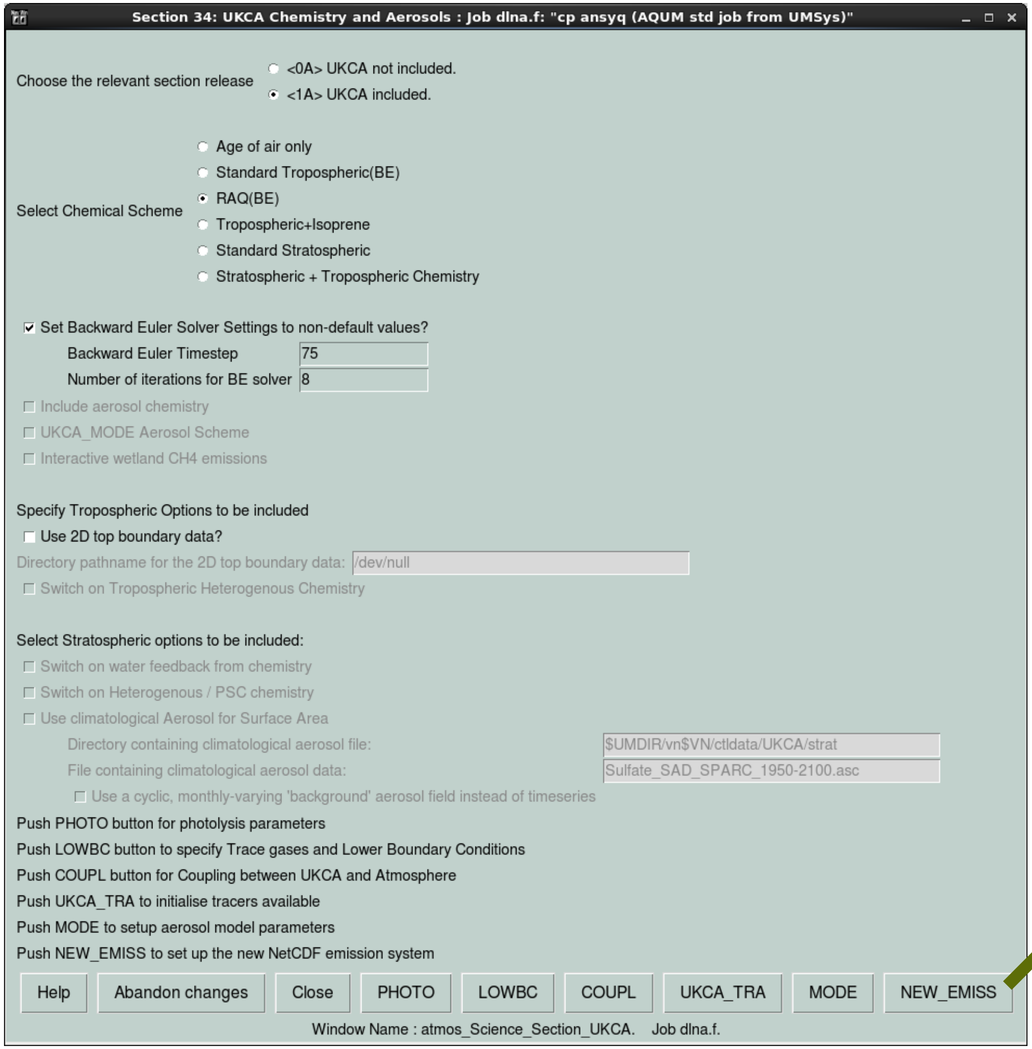
```
IF ( L_ukca_new_emiss )  THEN
         CALL ukca_new_emiss_ctl ( ... )
ELSE
         CALL UKCA_EMISSION_CTL  ( ... )
END IF
```

NetCDF (since UM vn8.6)

ancillaries

- **ukca_new_emiss_ctl.F90** includes calls to many routines in order to:
  - Go through NetCDF emission files to automatically identify emission fields present in them
  - Initialise an “emissions” structure which will hold all emission fields
  - Update the “emissions” structure when needed
  - Output emission diagnostics

NAMELIST input through UMUI (only available at UM vn8.6)


Section 34: UKCA Chemistry and Aerosols : Job dlna.f: "cp ansyq (AQUM std job from UMSys)"

Choose the relevant section release
○ <0A> UKCA not included.
● <1A> UKCA included.

Select Chemical Scheme
○ Age of air only
○ Standard Tropospheric(BE)
● RAQ(BE)
○ Tropospheric+Isoprene
○ Standard Stratospheric
○ Stratospheric + Tropospheric Chemistry

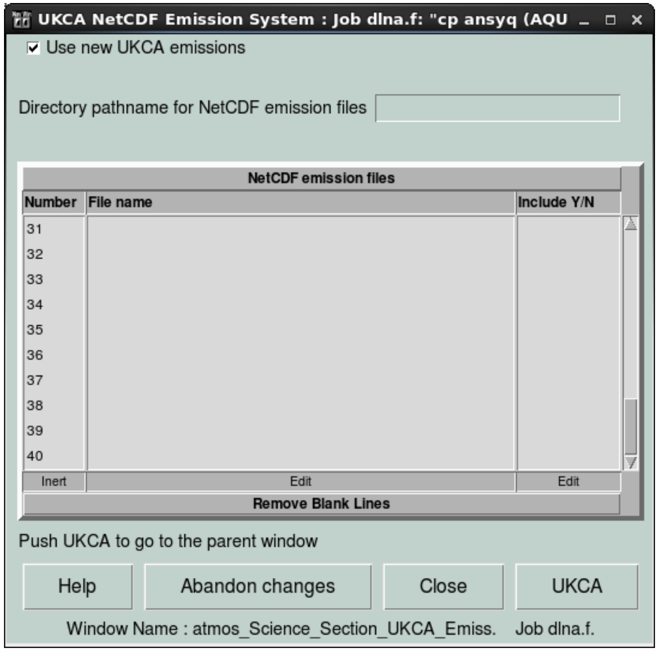
☑ Set Backward Euler Solver Settings to non-default values?
Backward Euler Timestep 75
Number of iterations for BE solver 8
□ Include aerosol chemistry
□ UKCA_MODE Aerosol Scheme
□ Interactive wetland CH4 emissions

Specify Tropospheric Options to be included
□ Use 2D top boundary data?
Directory pathname for the 2D top boundary data: /dev/null
□ Switch on Tropospheric Heterogenous Chemistry

Select Stratospheric options to be included:
□ Switch on water feedback from chemistry
□ Switch on Heterogenous / PSC chemistry
□ Use climatological Aerosol for Surface Area
Directory containing climatological aerosol file: $UMDIR/vn$VN/ctldata/UKCA/strat
File containing climatological aerosol data: Sulfate_SAD_SPARC_1950-2100.asc
□ Use a cyclic, monthly-varying 'background' aerosol field instead of timeseries

Push PHOTO button for photolysis parameters
Push LOWBC button to specify Trace gases and Lower Boundary Conditions
Push COUPL button for Coupling between UKCA and Atmosphere
Push UKCA_TRA to initialise tracers available
Push MODE to setup aerosol model parameters
Push NEW_EMISS to set up the new NetCDF emission system

Window Name : atmos_Science_Section_UKCA. Job dlna.f.



☑ Use new UKCA emissions

Directory pathname for NetCDF emission files

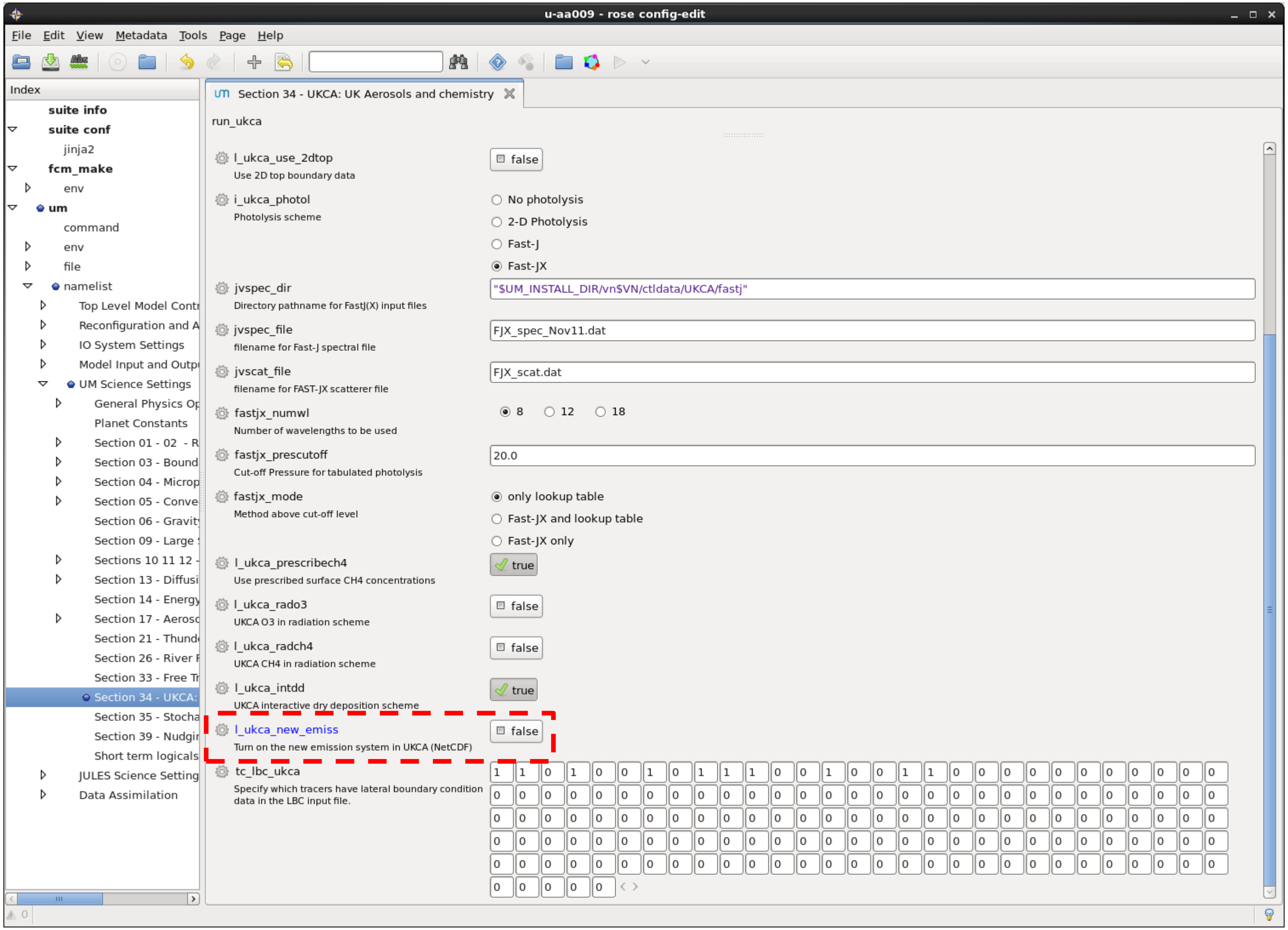
NetCDF emission files

Number	File name	Include Y/N
31		
32		
33		
34		
35		
36		
37		
38		
39		
40		

Push UKCA to go to the parent window

Window Name : atmos_Science_Section_UKCA_Emiss. Job dlna.f.

NAMELIST input through Rose (I)


u-aa009 - rose config-edit
File Edit View Metadata Tools Page Help
Index
Section 34 - UKCA: UK Aerosols and chemistry

- suite info
- suite conf
  - jinja2
- fcm_make
  - env
- um
  - command
  - env
  - file
  - namelist
    - Top Level Model Contr
    - Reconfiguration and A
    - IO System Settings
    - Model Input and Outp
    - UM Science Settings
      - General Physics Op
      - Planet Constants
      - Section 01 - 02 - R
      - Section 03 - Bound
      - Section 04 - Microp
      - Section 05 - Conve
      - Section 06 - Gravit
      - Section 09 - Large
      - Sections 10 11 12 -
      - Section 13 - Diffusi
      - Section 14 - Energy
      - Section 17 - Aeroso
      - Section 21 - Thund
      - Section 26 - River F
      - Section 33 - Free Tr
      - Section 34 - UKCA:
      - Section 35 - Stocha
      - Section 39 - Nudgi
      - Short term logicals
  - JULES Science Setting
  - Data Assimilation

run_ukca

l_ukca_use_2dtop
Use 2D top boundary data
□ false

i_ukca_photol
Photolysis scheme
○ No photolysis
○ 2-D Photolysis
○ Fast-J
● Fast-JX

jvspec_dir
Directory pathname for FastJ(X) input files
"$UM_INSTALL_DIR/vn$VN/ctldata/UKCA/fastj"

jvspec_file
filename for Fast-J spectral file
FJX_spec_Nov11.dat

jvscat_file
filename for FAST-JX scatterer file
FJX_scat.dat

fastjx_numwl
Number of wavelengths to be used
● 8 ○ 12 ○ 18

fastjx_prescutoff
Cut-off Pressure for tabulated photolysis
20.0

fastjx_mode
Method above cut-off level
● only lookup table
○ Fast-JX and lookup table
○ Fast-JX only

l_ukca_prescribech4
Use prescribed surface CH4 concentrations
✓ true

l_ukca_rado3
UKCA O3 in radiation scheme
□ false

l_ukca_radch4
UKCA CH4 in radiation scheme
□ false

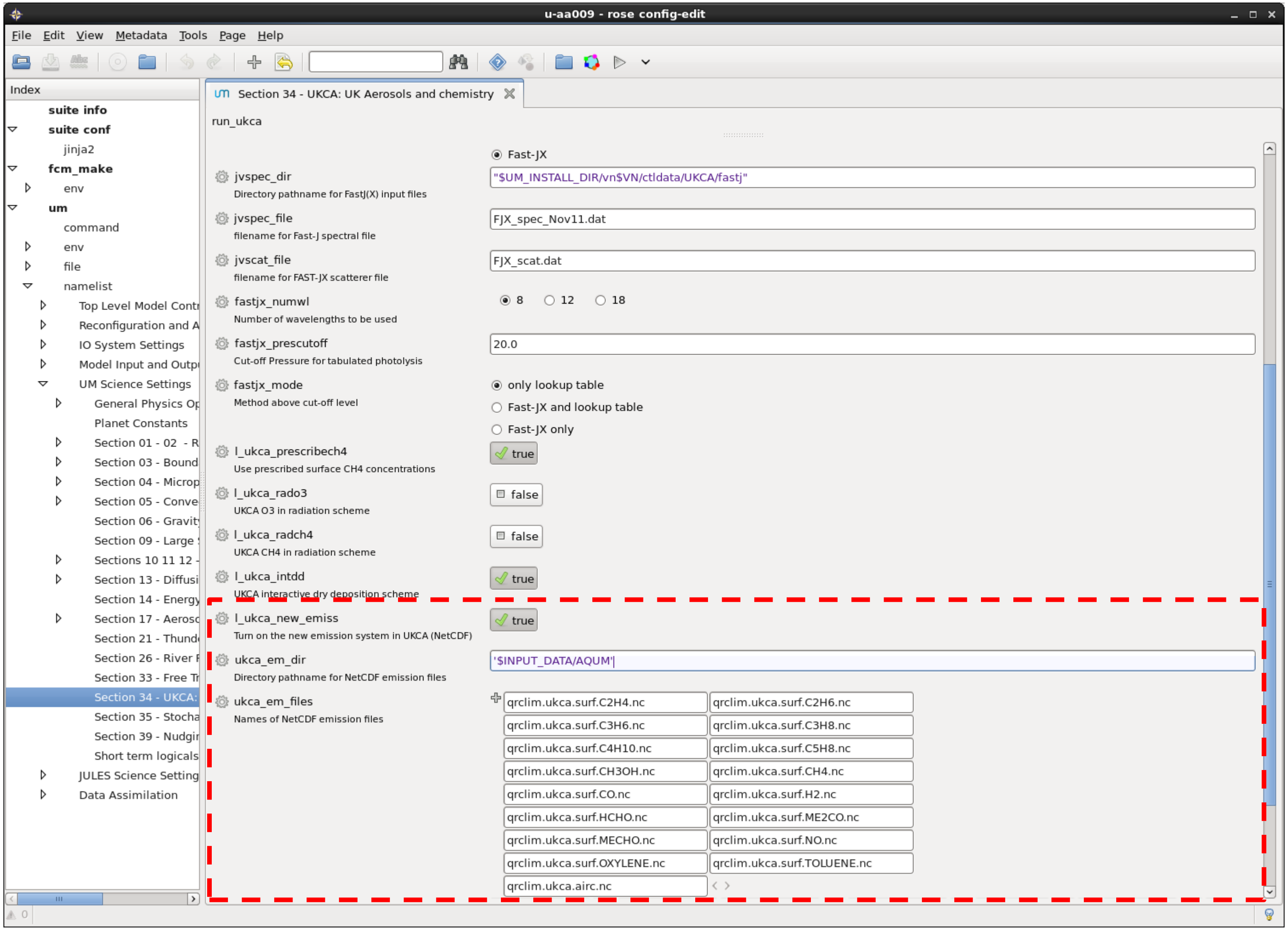
l_ukca_intdd
UKCA interactive dry deposition scheme
✓ true

l_ukca_new_emiss
Turn on the new emission system in UKCA (NetCDF)
□ false

tc_lbc_ukca
Specify which tracers have lateral boundary condition data in the LBC input file.

1	1	0	1	0	0	1	0	1	1	1	0	0	1	0	0	1	1	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0																								

NAMELIST input through Rose (II)



Section 34 - UKCA: UK Aerosols and chemistry

run_ukca

● Fast-JX

jvspec_dir
Directory pathname for FastJ(X) input files
"$UM_INSTALL_DIR/vn$VN/ctldata/UKCA/fastj"

jvspec_file
filename for Fast-J spectral file
FJX_spec_Nov11.dat

jvscat_file
filename for FAST-JX scatterer file
FJX_scat.dat

fastjx_numwl
Number of wavelengths to be used
● 8 ○ 12 ○ 18

fastjx_prescutoff
Cut-off Pressure for tabulated photolysis
20.0

fastjx_mode
Method above cut-off level
● only lookup table
○ Fast-JX and lookup table
○ Fast-JX only

l_ukca_prescribech4
Use prescribed surface CH4 concentrations
✓ true

l_ukca_rado3
UKCA O3 in radiation scheme
□ false

l_ukca_radch4
UKCA CH4 in radiation scheme
□ false

l_ukca_intdd
UKCA interactive dry deposition scheme
✓ true

l_ukca_new_emiss
Turn on the new emission system in UKCA (NetCDF)
✓ true

ukca_em_dir
Directory pathname for NetCDF emission files
'$INPUT_DATA/AQUM'

ukca_em_files
Names of NetCDF emission files

qrclim.ukca.surf.C2H4.nc	qrclim.ukca.surf.C2H6.nc
qrclim.ukca.surf.C3H6.nc	qrclim.ukca.surf.C3H8.nc
qrclim.ukca.surf.C4H10.nc	qrclim.ukca.surf.C5H8.nc
qrclim.ukca.surf.CH3OH.nc	qrclim.ukca.surf.CH4.nc
qrclim.ukca.surf.CO.nc	qrclim.ukca.surf.H2.nc
qrclim.ukca.surf.HCHO.nc	qrclim.ukca.surf.ME2CO.nc
qrclim.ukca.surf.MECHO.nc	qrclim.ukca.surf.NO.nc
qrclim.ukca.surf.OXYLENE.nc	qrclim.ukca.surf.TOLUENE.nc
qrclim.ukca.airc.nc	

Requirements of NetCDF files (1)

- **Maximum nr of emission files: 40**

ukca_option_mod.F90:

```
INTEGER, PARAMETER   :: nr_cdf_files = 40
CHARACTER (LEN=120) :: ukca_em_dir
CHARACTER(LEN=50)    :: ukca_em_files(nr_cdf_files)
```

Each NetCDF file may include one or several emission fields

- **Should comply with:**
  - **CF** conventions (http://cfconventions.org/)
  - **Met Office NetCDF** conventions

However UM code could still work if files don't comply.

- Next slides: **Metadata attributes** needed in the files so that the UM code works!

Requirements of NetCDF files (2)

Global attributes needed in **each emission file:**

- **update_freq_in_hours:** frequency in hours at which all emission fields present in that file should be read.

  If you want 5 days (as done for ancillaries in many UMUI jobs):

  update_freq_in_hours = 120

- **emission type** (follows same conventions as for ancillary files):
  - 0: Single time (not allowed yet)
  - 1: Time series
  - 2: Periodic time series

Requirements of NetCDF files (3)

Some **metadata attributes** required for **each emission field**:

- **name:** Name of the emission field (80 characters, only for debugging)

- **tracer_name:** This has to be equal to one of the names in the list of emissions for the given chemical scheme, i.e. **em_chem_spec**

- **standard_name** : Compulsory if available. Example for NO:

  `"tendency_of_atmosphere_mass_content_of_nitrogen_monoxide_due_to_emission"`

  `See http://cfconventions.org/Data/cf-standard-names/26/build/cf-standard-name-table.html`

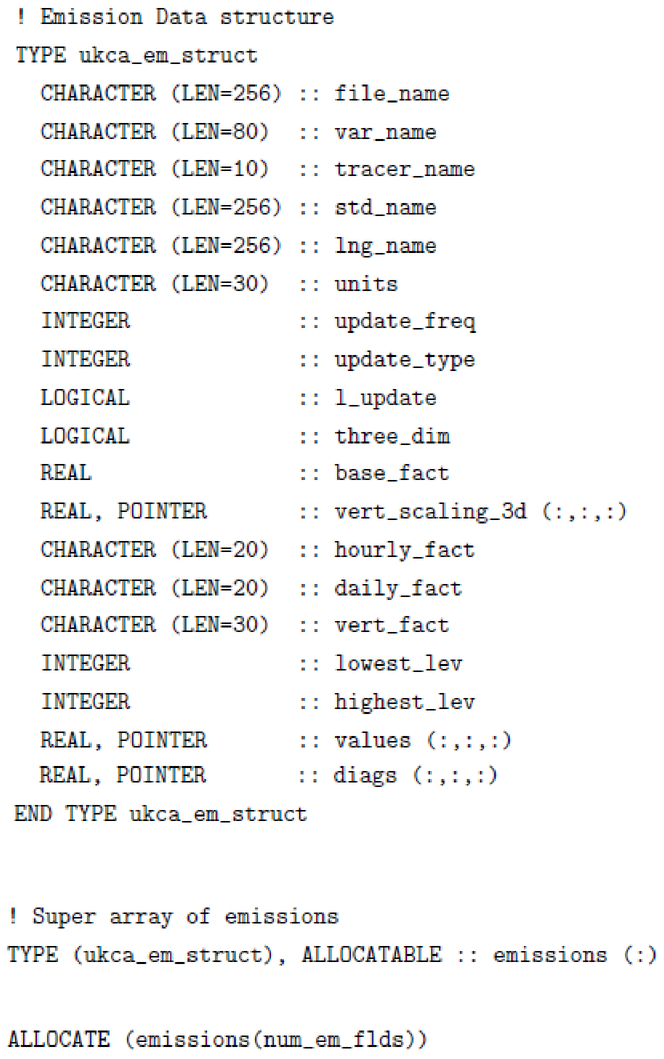
- **long_name:** Compulsory if there is no 'standard_name' available. Example:

  `"tendency of atmosphere mass content of nitrogen monoxide due to emission"`

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

- **hourly_scaling, daily_scaling & vertical_scaling:** Characters read by the UM to apply corresponding numeric scaling factors

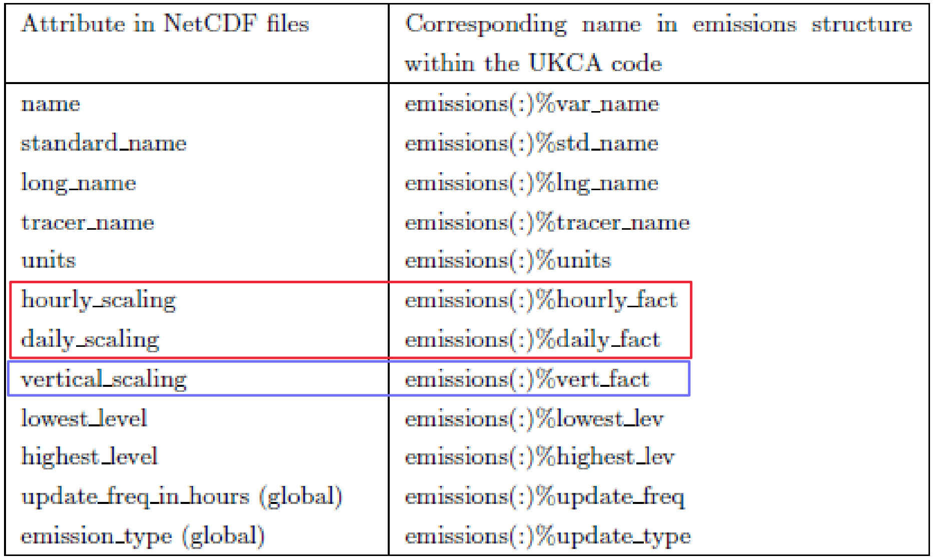
What UKCA code does with NetCDF attributes



```
! 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 (:)


ALLOCATE (emissions(num_em_flds))
```

1. The UKCA code creates an "emissions" structure (derived type variable) which contains objects representing emissions. Each object can be distinguished by some components: emission name, values, units, vertical/temporal profiles, ...

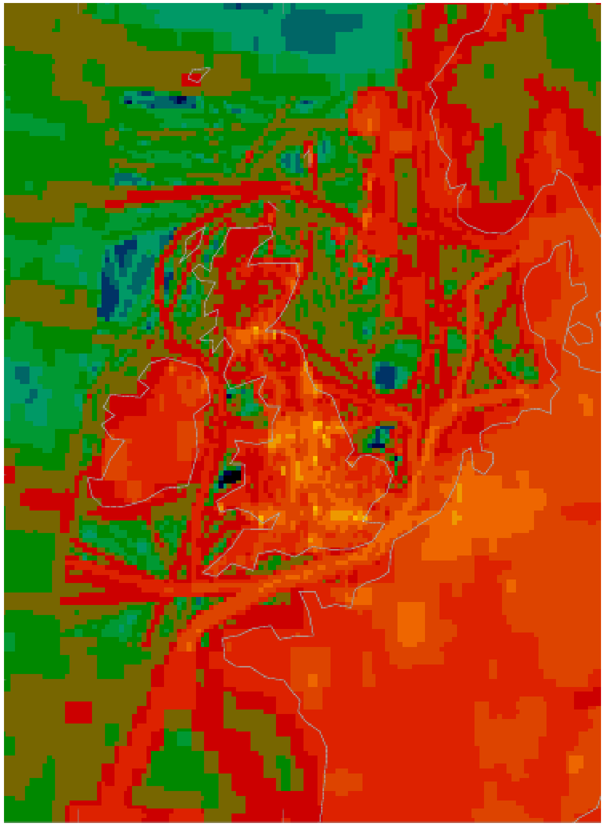
2. Then some of the NetCDF attributes are assigned to those components



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

Example of time / vertical profiles for RAQ (1)

Typical 12-monthly emission field for NO_x (all source sectors combined)



Better approach: Use separate SNAP source sectors

1 Combustion in energy and transformation industries

2 Non-industrial combustion plants

3 Combustion in manufacturing industry

4 Production processes

5 Extraction and distribution of fossil fuels

6 Solvents

7 Road transport (“traffic”)

8 Other mobile sources (e.g. shipping)

9 Waste treatment and disposal

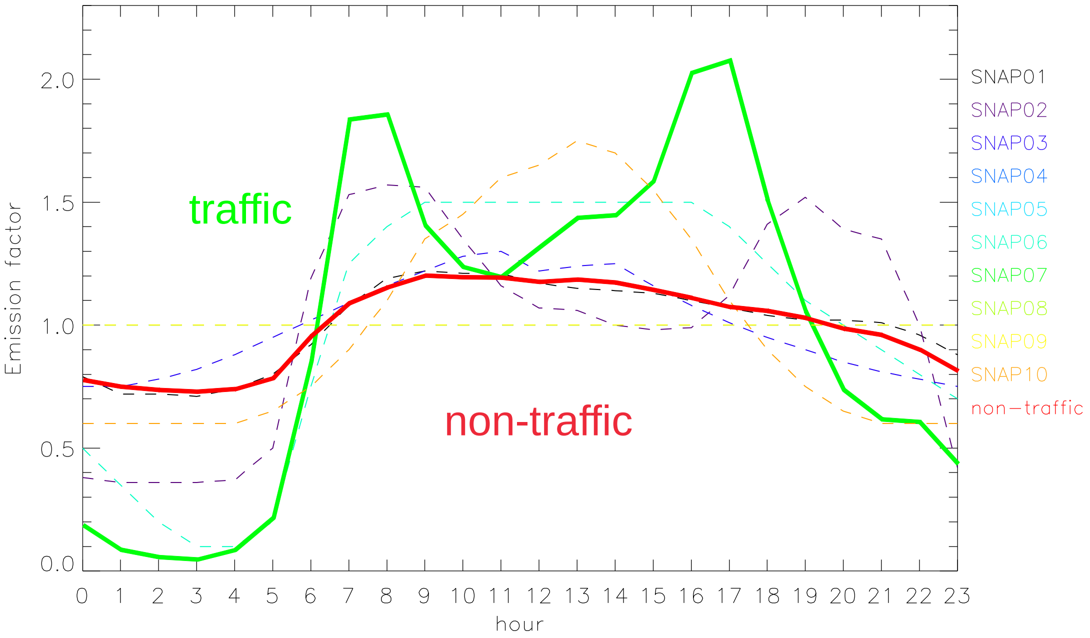
10 Agriculture

11 Natural and biogenic sources

Example of time / vertical profiles for RAQ (1a)

- **Hourly & daily factors** to account for daily and weekly variability in emissions
- Based on data provided by TNO for the MACC project

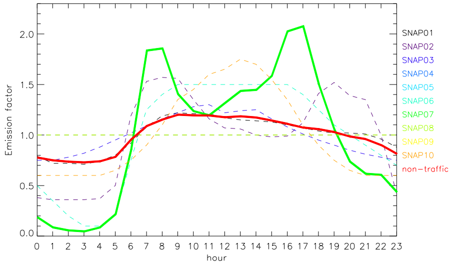
Hourly factors



Example of time / vertical profiles for RAQ (1b)

Module UKCA_EMISS_FACTORS - Subroutine HOURLY_EMISS_FACTORS

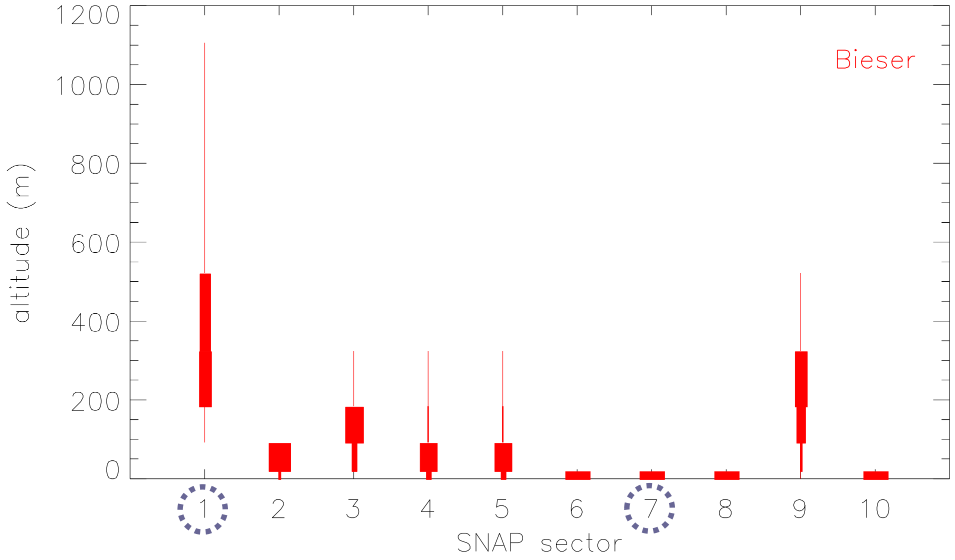
```
SELECT CASE (TRIM (hourly_fact))    ← NetCDF attribute hourly_scaling

    ! No hourly factors applied unless specified
    CASE ('none', '')
      hourly_scaling =                                                &
         (/1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00,     &
           1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00,     &
           1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00, 1.00/)


    ! ---------------------------------------------------------------------
    ! Hourly factors of emissions for Europe. Calculated by TNO
    ! for the MACC project.

    ...

    CASE ('TNO_MACC_EU_SNAP07')
      hourly_scaling =                                                &
         (/0.19, 0.09, 0.06, 0.05, 0.09, 0.22, 0.86, 1.84,     &
           1.86, 1.41, 1.24, 1.20, 1.32, 1.44, 1.45, 1.59,     &
           2.03, 2.08, 1.51, 1.06, 0.74, 0.62, 0.61, 0.44/)
   ...

END SELECT
```



Example of time / vertical profiles for RAQ (2a)

Vertical profiles tested for anthropogenic emissions in RAQ chemistry scheme

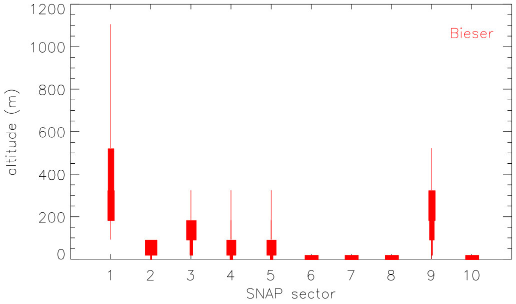
Vertical disaggregation for SNAP sectors 1–10



Example of time / vertical profiles for RAQ (2b)

Module UKCA_EMISS_FACTORS - Subroutine VERTICAL_EMISS_FACTORS

```
! Altitude of the interfaces in metres
interf_ref = (/0.0, 20.0, 92.0, 184.0, 324.0, 522.0, 781.0, 1106.0/)

! Get a 3D vertical scaling factor for the given profile
  SELECT CASE (TRIM (vert_fact)) ← NetCDF attribute vertical_scaling

!   Average vertical profiles for various SNAP source sectors.
    CASE ('Bieser_modified_SNAP01')
      vert_scaling_ref (:) = (/  0.0,   0.0, 0.25, 51.0, 45.3, 3.25, 0.2 /)

    ...

    CASE ('Bieser_modified_SNAP07')
      vert_scaling_ref (:) = (/ 100.0,   0.0,   0.0,   0.0,   0.0,   0.0,   0.0 /)

    ...


    ! Surface emiss in lowest model lev unless something different specified
    CASE ('surface', '')
      vert_scaling_3d (:, :, 1)    = 1.0
      vert_scaling_3d (:, :, 2:)   = 0.0

    ! 3D emissions over all model levels
    CASE ('all_levels', '3D')
      vert_scaling_3d (:,:,:)    = 1.0
    ...

 END SELECT
```



How to deal with special units

- **Attribute units in all NetCDF emission fields:**

  units = “kg m-2 s-1”   or   units = “kg/m2/s”

- **If you want to express in kg(N), kg(C) or kg(S):**

standard_name = “tendency_of_atmosphere_mass_content_of_**nox**_**expressed_as_nitrogen**_due_to_emission”

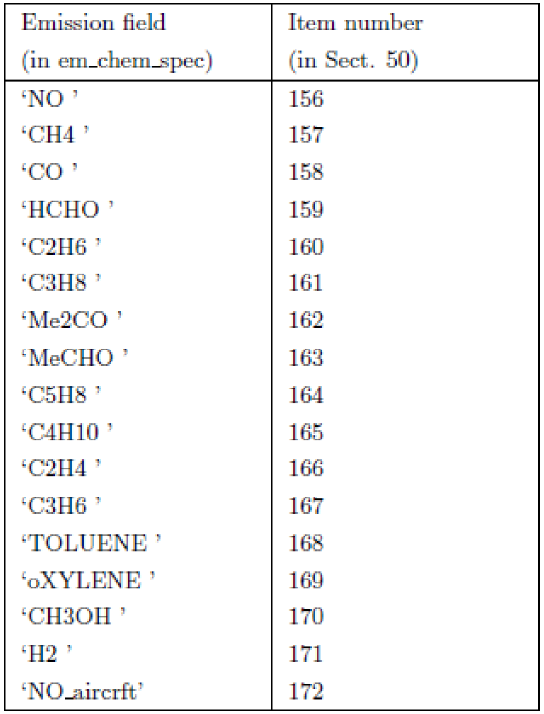
Check http://cfconventions.org/Data/cf-standard-names/27/build/cf-standard-name-table.html

long_name = “tendency of atmosphere mass content of **isoprene** **expressed as carbon** due to emission”

- See code in 2 routines within the module **ukca_emiss_factors**:
  - Strings automatically detected by **base_emiss_factors**
  - Conversions done in **get_base_scaling**

  You might need to adapt them

New emission diagnostics (1)



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

- Available for RAQ & other schemes
- New items can be added in S50

ukca_add_emiss_mod.F90

emissions(l)%diags (:, :,1) filled

Column integrated & with time profiles applied

ukca_emdiags_struct_modF90:

Declares a structure for emission diagnostics:

```
TYPE emdiags_struct
   ! Flags indicating if diagnostics selected
   LOGICAL :: l_em_no
   LOGICAL :: l_em_ch4
   ...

   ! Pointers to hold emission diagnostics
   REAL, POINTER :: em_no     (:,:)
   REAL, POINTER :: em_ch4    (:,:)
   ...
   REAL, POINTER :: em_no_air (:,:,:)
END TYPE emdiags_struct
```

ukca_update_emdiagstruct_mod.F90

Update emission diagnostic values and flags in the "emdiags_struct"

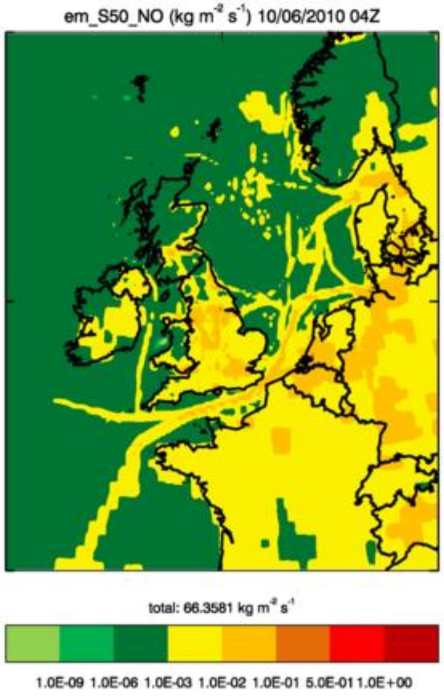
ukca_emiss_diags_mod.F90

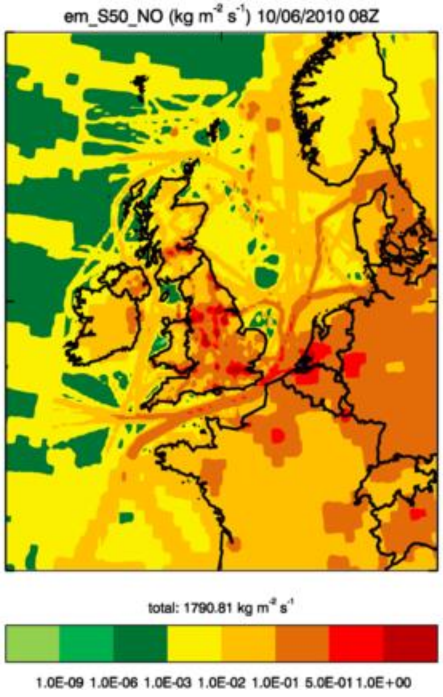
Output emission diagnostics

New emission diagnostics (2)

Emission diagnostics for NO:

1. With temporal factors applied
2. Column integrated (always for 2-D emissions)
3. In kg (NO) m^{-2} s^{-1}


em_S50_NO (kg m-2 s-1) 10/06/2010 04Z
total: 66.3581 kg m-2 s-1
1.0E-09 1.0E-06 1.0E-03 1.0E-02 1.0E-01 5.0E-01 1.0E+00


em_S50_NO (kg m-2 s-1) 10/06/2010 08Z
total: 1790.81 kg m-2 s-1
1.0E-09 1.0E-06 1.0E-03 1.0E-02 1.0E-01 5.0E-01 1.0E+00

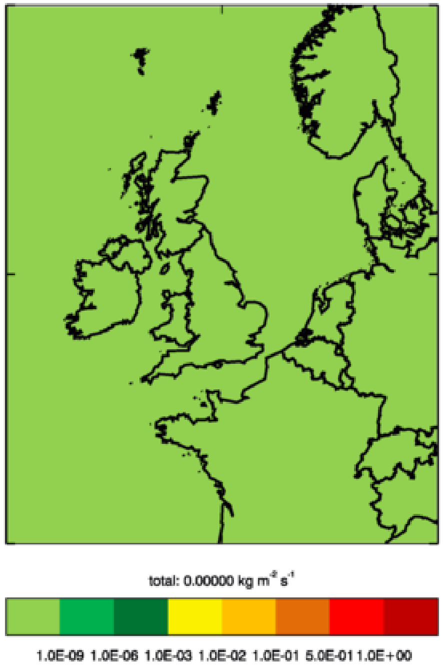
New emission diagnostics (3)

Emission diagnostics for (non-interactive) **isoprene emissions,** with netCDF attributes:

```
        tracer_name    = ‘C5H8’
        hourly_scaling = ‘diurnal_isopems’
```

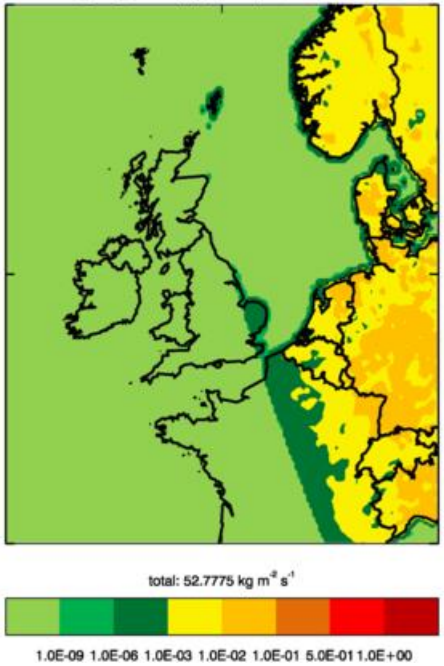
➔ diurnal cycle applied via call to **ukca_diurnal_isop_ems.F90**

em_S50_C5H8 (kg m^{-2} s^{-1}) 10/06/2010 04Z



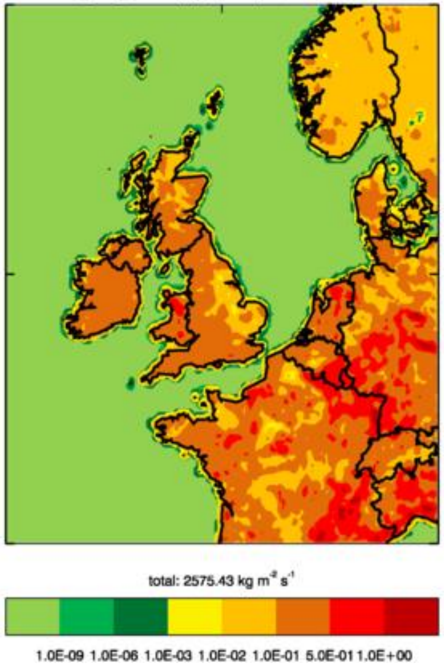
total: 0.00000 kg m^{-2} s^{-1}

em_S50_C5H8 (kg m^{-2} s^{-1}) 10/06/2010 06Z



total: 52.7775 kg m^{-2} s^{-1}

em_S50_C5H8 (kg m^{-2} s^{-1}) 10/06/2010 12Z



total: 2575.43 kg m^{-2} s^{-1}

NetCDF emission system will be extended for iBVOC emissions of C_5H_8 and other species

ukca_new_emiss_ctl.F90 (1)

```
IF ( l_first )  THEN

   ! Read emission NetCDF files and look for the the emission fields
   ! in them to allocate all variables in the emissions structure.
   CALL ukca_emiss_init (…)

   ! Get scaling factors indicating how to to spread emissions
   ! over different vertical levels. Done it only once here and
   ! stored in the emissions structure, then valid for all time steps.
   DO l = 1, num_em_flds
       CALL vertical_emiss_factors   (...,  vert_fact_3d)
       emissions(l)%vert_scaling_3d (:,:,:) = vert_fact_3d (:,:,:)
   END DO

END IF
```

```
! ---------------------------------------------------------------------------
! Check if it is time to update the emiss fields that
! we read from NetCDF files (depending on time step
! and update frequency). If needed then update the files.

CALL ukca_emiss_update (…)
```

! ---
! **Deal with online emissions**. Always updated at each time step
! For the moment only NO_x from lightning and CH_4 from wetlands

ukca_new_emiss_ctl.F90 (2)

```
! -----------------------------------------------------------------------------------------
! Update all fields in the emissions super array:
! * Do conversions so that emissions are given as 'kg(tracer) m-2 s-1'
! * Update isoprene emissions if they are diurnally varying

DO l = 1, num_em_flds

   IF (emissions(l)%l_update) THEN

      CALL base_emiss_factors

      update “emissions(l)%values“

   END IF


   For isoprene: CALL ukca_diurnal_isop_ems
                  to apply diurnal cycle

END DO



-----------------------------------------------------
! Inject emissions and do tracer mixing
CALL ukca_add_emiss ( …)



! ---------------------------------------------------------------------------------------
! Call the emission diagnostics code if any of the diagnostics present
! in the routine GET_EMDIAG_STASH has been selected via stash.

 CALL ukca_emiss_diags (...)
```

4. Final notes

Final notes

- This talk is based on UM vn9.2. Some functionalities not available for older UM versions.
- I have not covered some topics in detail (aerosol emissions, BVOC emissions, ...).

Useful reading material

- **Online UKCA tutorial**

  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorial_5

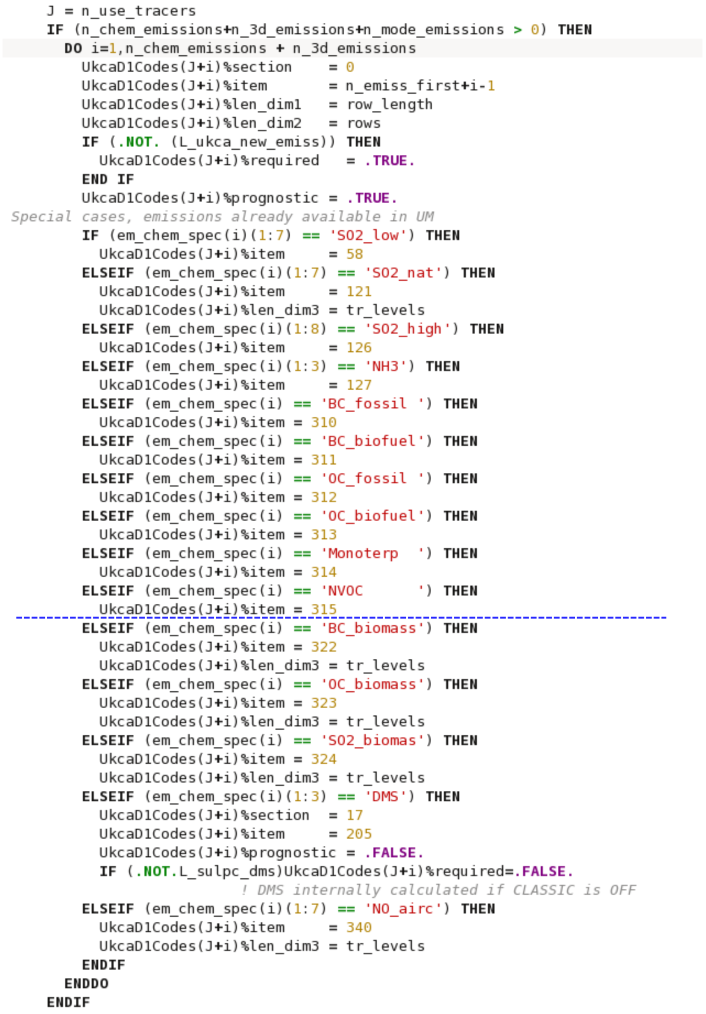
- **UKCA - UMDP 84**
  - Chapter 10: Emissions (ancillary system)
  - Chapter 11: New NetCDF emission system

    https://code.metoffice.gov.uk/doc/um/vn9.2/umdp.html
    https://code.metoffice.gov.uk/doc/um/vn10.0/umdp.html

Met Office

Code in ukca_setd1defs.F90

Complicated block of code further down in this routine



```
    J = n_use_tracers
    IF (n_chem_emissions+n_3d_emissions+n_mode_emissions > 0) THEN
      DO i=1,n_chem_emissions + n_3d_emissions
        UkcaD1Codes(J+i)%section    = 0
        UkcaD1Codes(J+i)%item       = n_emiss_first+i-1
        UkcaD1Codes(J+i)%len_dim1   = row_length
        UkcaD1Codes(J+i)%len_dim2   = rows
        IF (.NOT. (L_ukca_new_emiss)) THEN
          UkcaD1Codes(J+i)%required   = .TRUE.
        END IF
        UkcaD1Codes(J+i)%prognostic = .TRUE.
Special cases, emissions already available in UM
        IF (em_chem_spec(i)(1:7) == 'SO2_low') THEN
          UkcaD1Codes(J+i)%item     = 58
        ELSEIF (em_chem_spec(i)(1:7) == 'SO2_nat') THEN
          UkcaD1Codes(J+i)%item     = 121
          UkcaD1Codes(J+i)%len_dim3 = tr_levels
        ELSEIF (em_chem_spec(i)(1:8) == 'SO2_high') THEN
          UkcaD1Codes(J+i)%item     = 126
        ELSEIF (em_chem_spec(i)(1:3) == 'NH3') THEN
          UkcaD1Codes(J+i)%item     = 127
        ELSEIF (em_chem_spec(i) == 'BC_fossil ') THEN
          UkcaD1Codes(J+i)%item = 310
        ELSEIF (em_chem_spec(i) == 'BC_biofuel') THEN
          UkcaD1Codes(J+i)%item = 311
        ELSEIF (em_chem_spec(i) == 'OC_fossil ') THEN
          UkcaD1Codes(J+i)%item = 312
        ELSEIF (em_chem_spec(i) == 'OC_biofuel') THEN
          UkcaD1Codes(J+i)%item = 313
        ELSEIF (em_chem_spec(i) == 'Monoterp  ') THEN
          UkcaD1Codes(J+i)%item = 314
        ELSEIF (em_chem_spec(i) == 'NVOC      ') THEN
          UkcaD1Codes(J+i)%item = 315
        ELSEIF (em_chem_spec(i) == 'BC_biomass') THEN
          UkcaD1Codes(J+i)%item = 322
          UkcaD1Codes(J+i)%len_dim3 = tr_levels
        ELSEIF (em_chem_spec(i) == 'OC_biomass') THEN
          UkcaD1Codes(J+i)%item = 323
          UkcaD1Codes(J+i)%len_dim3 = tr_levels
        ELSEIF (em_chem_spec(i) == 'SO2_biomas') THEN
          UkcaD1Codes(J+i)%item = 324
          UkcaD1Codes(J+i)%len_dim3 = tr_levels
        ELSEIF (em_chem_spec(i)(1:3) == 'DMS') THEN
          UkcaD1Codes(J+i)%section  = 17
          UkcaD1Codes(J+i)%item     = 205
          UkcaD1Codes(J+i)%prognostic = .FALSE.
          IF (.NOT.L_sulpc_dms)UkcaD1Codes(J+i)%required=.FALSE.
                          ! DMS internally calculated if CLASSIC is OFF
        ELSEIF (em_chem_spec(i)(1:7) == 'NO_airc') THEN
          UkcaD1Codes(J+i)%item     = 340
          UkcaD1Codes(J+i)%len_dim3 = tr_levels
        ENDIF
      ENDDO
    ENDIF
```

Meaning

- STASH 301–309 in same order as **em_chem_spec**
- STASH items defined for some emissions (e.g. items 322, 323, 324 reserved for 3D emissions)

Main thing to remember:

- single-level: items 301-320
- multi-level: items 321-340