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\textsubscript{x}
  - Sea-salt (in GLOMAP-mode)
  - Wetland CH\textsubscript{4} (from JULES)
  - Interactive BVOC (from JULES; for isoprene, terpenes, methanol, acetone; since UM vn9.2).
## Gas phase emissions

<table>
<thead>
<tr>
<th>Emission Species</th>
<th>Units</th>
<th>Std Trop</th>
<th>Trop-Isop</th>
<th>RAQ Chem</th>
<th>Strat Chem</th>
<th>Strat+Trop</th>
</tr>
</thead>
<tbody>
<tr>
<td>NOx Surface Emissions</td>
<td>kg(NO2)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>CH4 Surface Emissions</td>
<td>kg(CH4)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>CO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>HCHO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>C2H6 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>C3H8 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>CH3COCH3 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>CH3CHO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>C5H8 (Isop) Surface Emiss</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
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<tr>
<td>H2 Surface Emissions</td>
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<tr>
<td>C3H6 Surface Emissions</td>
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<tr>
<td>Toluene Surface Emissions</td>
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<tr>
<td>o-xylene Surface Emissions</td>
<td>kg/m²/s</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>CH3OH Surface Emissions</td>
<td>kg(C)/m²/s</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NOx Aircraft Emissions (3D)</td>
<td>kg(NO2)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
</tbody>
</table>

(Taken from UMDP 084 for UKCA)
# Aerosol & online emissions

<table>
<thead>
<tr>
<th>Emission Species</th>
<th>Units</th>
<th>Std Trop</th>
<th>Trop-Isopt</th>
<th>RAQ Chem</th>
<th>Strat Chem</th>
<th>Strat+ Trop</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>If using Aerosol Chem</strong></td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Monoterpene Surface Emiss</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>NVOC Surface Emiss</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>SO2 Surface Emissions</td>
<td>kg(S)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DMS Surf Emiss (Land,ocean)</td>
<td>kg(S)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td>Y</td>
</tr>
<tr>
<td>NH3 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>C</td>
<td>Y</td>
</tr>
<tr>
<td>SO2 High (Ind,forest,ship)</td>
<td>kg(S)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>SO2 Volcanic Emissions (3D)</td>
<td>kg(S)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>C</td>
<td></td>
</tr>
<tr>
<td><strong>for GLOMAP-mode (if using 5-mode setup)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BC Fossil Fuel Emiss</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OC Fossil Fuel Emiss</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BC Biofuel Emissions</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OC Biofuel Emissions</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td>C</td>
<td></td>
</tr>
<tr>
<td>BC Biomass burn Emiss (3D)</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>OC Biomass burn Emiss (3D)</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
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<td></td>
<td></td>
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<tr>
<td><strong>Online Emissions</strong></td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>CH4 Wetland Emiss (in LSH - Optional)</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Lightning NOx (in UKCA)</td>
<td>kg(NO2)/kg(air)/cell/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>Sea-Salt Emiss (in GLOMAP-mode)</td>
<td>number/m²/s</td>
<td>Y</td>
<td>Y</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

(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)

Rest of items in section 0 reserved for UM prognostics

<table>
<thead>
<tr>
<th>STASH code</th>
<th>Emission Species</th>
<th>Units</th>
<th>Std Trop</th>
<th>Trop-Iso</th>
<th>RAQ Chem</th>
<th>Strat Chem</th>
<th>Strat+ Trop</th>
</tr>
</thead>
<tbody>
<tr>
<td>301</td>
<td>NOx Surface Emissions</td>
<td>kg(NO2)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>302</td>
<td>CH4 Surface Emissions</td>
<td>kg(CH4)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>303</td>
<td>CO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>304</td>
<td>HCHO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>305</td>
<td>C2H6 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>306</td>
<td>C3H8 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>307</td>
<td>CH3COCH3 Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>308</td>
<td>CH3CHO Surface Emissions</td>
<td>kg/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td>309</td>
<td>C5H8 (Isop) Surface Emissions</td>
<td>kg(C)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
<tr>
<td></td>
<td>NOx Aircraft Emissions (3D)</td>
<td>kg(NO2)/m²/s</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
<td>Y</td>
</tr>
</tbody>
</table>
Need to add STASH items

#
1| 1 | 0 | 301 | NOx surf emissions |
2| 2 | 0 | 1 | 1 | 5 | -1 | -1 | 0 | 0 | 0 | 0 |
3| 000000000000000000000000000000000000000001 | 3 |
5| 0 | 531 | 0 | 129 | 0 | 0 | 0 | 0 | 0 |
#

#
1| 1 | 0 | 340 | NOX AIRCRAFT EMS IN KG/S/GRIDCELL |
2| 2 | 0 | 1 | 1 | 2 | 10 | 11 | 0 | 0 | 0 | 0 |
3| 000000000000000000000000000000000000000001 | 3 |
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_aircraft' /)

  NOx emissions: Expressed as kg(NO₂) m⁻² s⁻¹ but assigned to the NO tracer!
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' /)

NOx emissions: Expressed as kg(NO2) 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)
Both cases accept online emissions
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
  CALL ukca\_mode\_ems\_um ! Number & mass emission fluxes are assembled for each tracer
END IF

! **Regrid interactive 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 …
! 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
    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

! 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
! 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 (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

! 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
! 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
! 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
! Check if tracer has **surface emissions** and set emission. Otherwise emission field is zero from initialisation.

DO k = 1, jpcrt  ! loop over tracers
  DO l = 1, n_chem_emissions
    !
    ! Convert from kg NO2/m2/s to kg NO/m2/s
    !
    !            Convert from kg NO2/m2/s to kg NO/m2/s
    !
    !            Convert from kg NO2/m2/s to kg NO/m2/s
    !
    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
      !
      else if advt(k) == em_chem_spec(l) THEN
      !
      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
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_emissions_um  \rightarrow em_field_mode is filled with nr & mass emission fluxes for each tracer
END IF

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

2. CALL ukca_mode_emissions: 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 ACCUMULATION (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) |
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_emis_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
! Beginning of ukca_emission_ctl. Call routine for primary emissions for UKCA-MODE
IF (L_ukca_mode) THEN
    CALL ukca_mode_emss_um  \(\Rightarrow\) em_field_mode is filled with nr & mass emission fluxes for each tracer
END IF

! 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
! 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
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`:

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

• `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)
NAMELIST input through Rose (I)
NAMELIST input through Rose (II)
Requirements of NetCDF files (1)

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

  ukca_option_mod.F90:
  
  ```fortran
  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/](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!
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”


- **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

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

<table>
<thead>
<tr>
<th>Attribute in NetCDF files</th>
<th>Corresponding name in emissions structure within the UKCA code</th>
</tr>
</thead>
<tbody>
<tr>
<td>name</td>
<td>emissions(:)%var_name</td>
</tr>
<tr>
<td>standard_name</td>
<td>emissions(:)%std_name</td>
</tr>
<tr>
<td>long_name</td>
<td>emissions(:)%lng_name</td>
</tr>
<tr>
<td>tracer_name</td>
<td>emissions(:)%tracer_name</td>
</tr>
<tr>
<td>units</td>
<td>emissions(:)%units</td>
</tr>
<tr>
<td>hourly_scaling</td>
<td>emissions(:)%hourly_fact</td>
</tr>
<tr>
<td>daily_scaling</td>
<td>emissions(:)%daily_fact</td>
</tr>
<tr>
<td>vertical_scaling</td>
<td>emissions(:)%vert_fact</td>
</tr>
<tr>
<td>lowest_level</td>
<td>emissions(:)%lowest_lev</td>
</tr>
<tr>
<td>highest_level</td>
<td>emissions(:)%highest_lev</td>
</tr>
<tr>
<td>update_freq_in_hours (global)</td>
<td>emissions(:)%update_freq</td>
</tr>
<tr>
<td>emission_type (global)</td>
<td>emissions(:)%update_type</td>
</tr>
</tbody>
</table>
Typical 12-monthly emission field for NO\textsubscript{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
• **Hourly & daily factors** to account for daily and weekly variability in emissions

• Based on data provided by TNO for the MACC project
Module UKCA_EMISS_FACTORS - Subroutine HOURLY_EMISS_FACTORS

SELECT CASE (TRIM (hourly_fact))
    ! 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
Vertical profiles tested for anthropogenic emissions in RAQ chemistry scheme.
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”
  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)

**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:

```fortran
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

---

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

• Available for RAQ & other schemes

• New items can be added in S50
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$^{-1}$
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

NetCDF emission system will be extended for iBVOC emissions of C$_5$H$_8$ and other species
IF ( _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\textsubscript{x} from lightning and CH\textsubscript{4} from wetlands
! 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 $l = 1, \text{num\_em\_filds}$

    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 (...)

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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](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/vn10.0/umdp.html](https://code.metoffice.gov.uk/doc/um/vn10.0/umdp.html)
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

Complicated block of code further down in this routine...

```
J = n_use_tracers
IF (n_chem_emissions+3D_emissions+n_node_emissions > 0) THEN
  DO i=n_chem_emissions+3D_emissions
     Ukca01Codes(i)%i%section = 0
     Ukca01Codes(i)%i%item = n_emiss_first+i-1
     Ukca01Codes(i)%i%len_dim = row_length
     Ukca01Codes(i)%i%len_dim2 = rows
     IF (.NOT. (L_ukca_new_emiss)) THEN
         Ukca01Codes(i)%i%required = .TRUE.
     END IF
   Ukca01Codes(i)%i%prognostic = .TRUE.
   Special cases, emissions already available in UM
   IF (em_chem_spec(i)(1:1) == 'SO2_low') THEN
       Ukca01Codes(i)%i%item = 90
   ELSEIF (em_chem_spec(i)(1:7) == 'SO2_nat') THEN
       Ukca01Codes(i)%i%item = 121
   ELSEIF (em_chem_spec(i)(1:8) == 'SO2_high') THEN
       Ukca01Codes(i)%i%item = 120
   ELSEIF (em_chem_spec(i)(1:3) == 'NH3') THEN
       Ukca01Codes(i)%i%item = 127
   ELSEIF (em_chem_spec(i) == 'BC_fossil') THEN
       Ukca01Codes(i)%i%item = 310
   ELSEIF (em_chem_spec(i) == 'BC_biofuel') THEN
       Ukca01Codes(i)%i%item = 311
   ELSEIF (em_chem_spec(i) == 'OC_fossil') THEN
       Ukca01Codes(i)%i%item = 332
   ELSEIF (em_chem_spec(i) == 'OC_biofuel') THEN
       Ukca01Codes(i)%i%item = 333
   ELSEIF (em_chem_spec(i) == 'Monoterp ') THEN
       Ukca01Codes(i)%i%item = 334
   ELSEIF (em_chem_spec(i) == 'NOx') THEN
       Ukca01Codes(i)%i%item = 312
   ELSEIF (em_chem_spec(i) == 'BC_biomass') THEN
       Ukca01Codes(i)%i%item = 322
   ELSEIF (em_chem_spec(i) == 'OC_biomass') THEN
       Ukca01Codes(i)%i%item = 323
   ELSEIF (em_chem_spec(i) == 'SO2_biomass') THEN
       Ukca01Codes(i)%i%item = 324
   ELSEIF (em_chem_spec(i)(1:3) == 'DMS') THEN
       Ukca01Codes(i)%i%item = 205
   ELSEIF (em_chem_spec(i)(1:7) == 'NO_airc') THEN
       Ukca01Codes(i)%i%item = 346
   ENDIF
   ENDIF
ENDIF
```