UKCA Theory and Practice 2018

Emissions in UKCA

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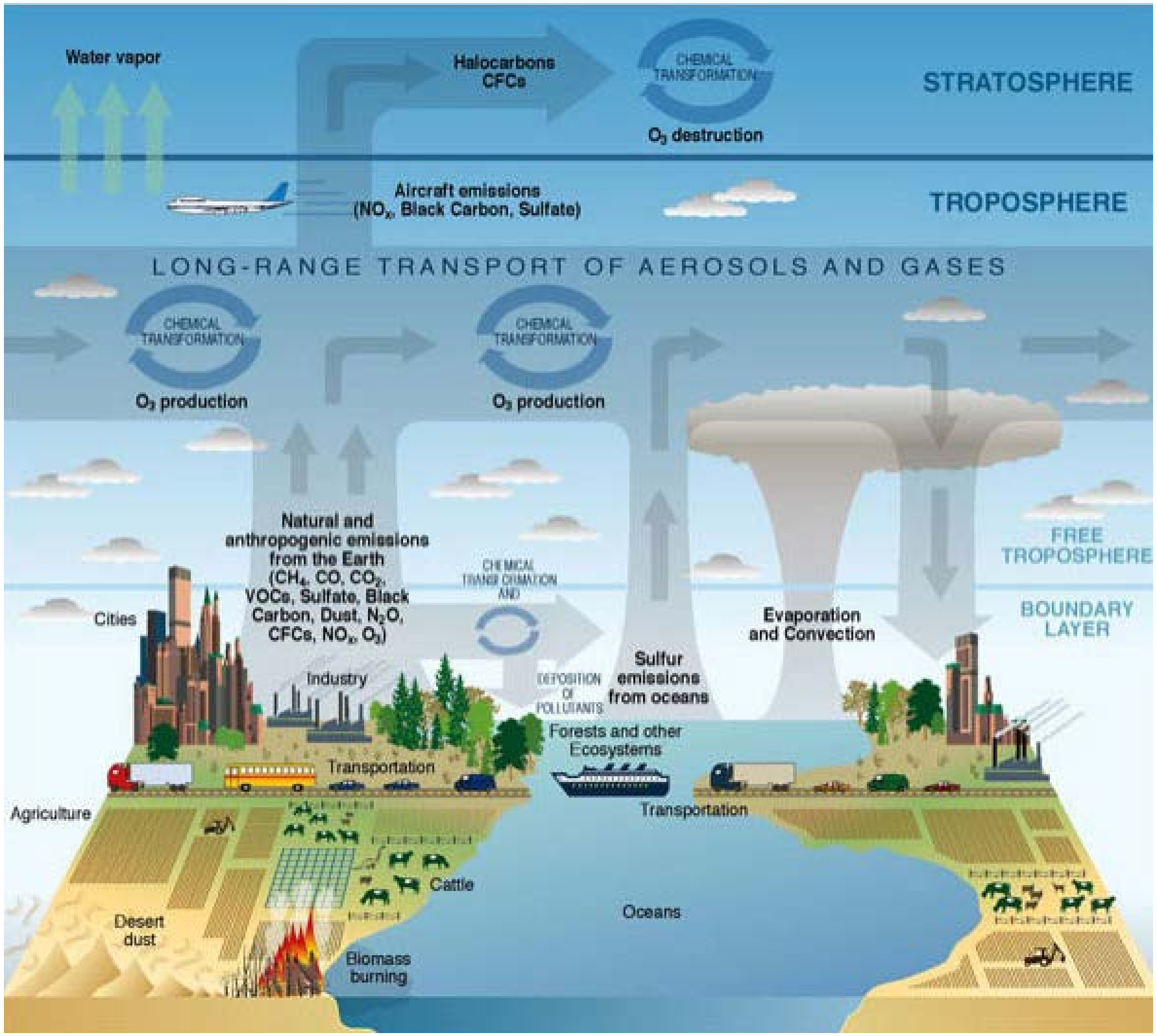
with liberally borrowed material from earlier course presentations from 2015–2017 by Dr Alex Archibald and Dr Carlos Ordóñez

Role of Emissions in Global Atmospheric Chemistry

- Primary release mechanism of reactive chemical compounds into the atmosphere

- In global chemistry modelling emissions have a major impact on calculated results

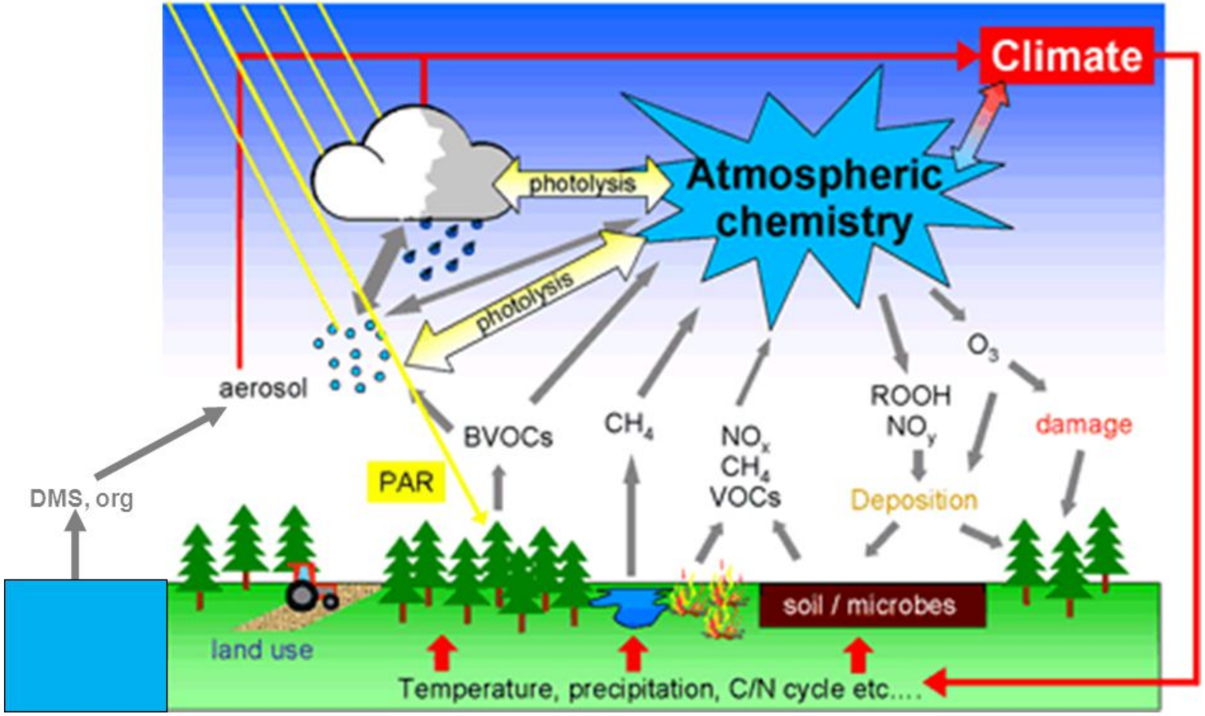
- All model users will work with emissions at some stage.



Emissions Classification

- What types of emissions exist?
  - Natural sources
  - Anthropogenic sources
  - Classification by other criteria, e.g. gas phase versus aerosol

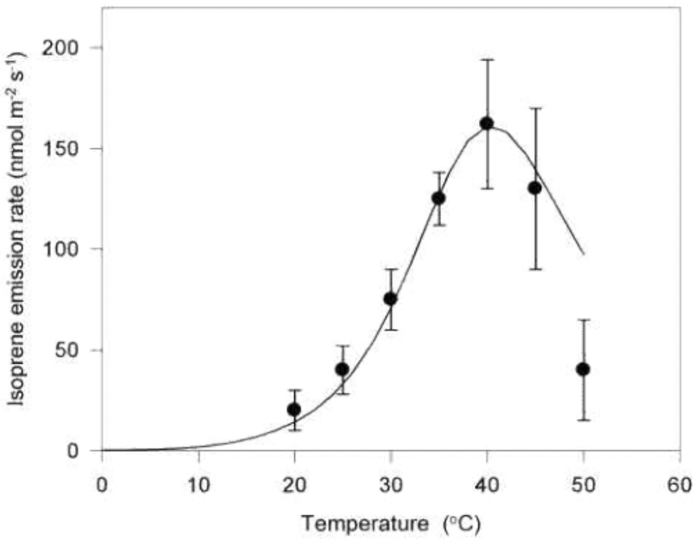
AN ATMOSPHERIC CHEMISTRY PERSPECTIVE...

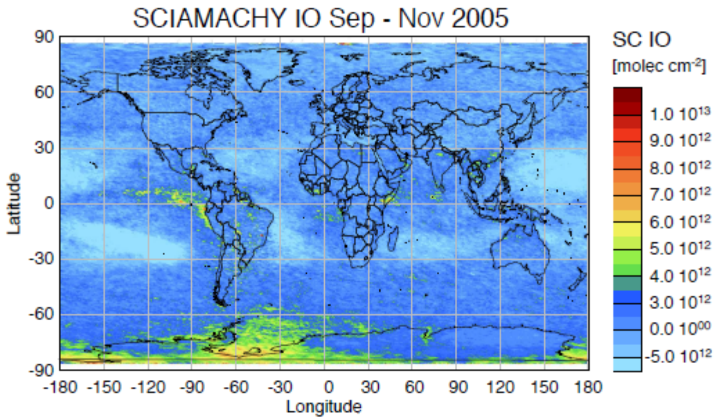


From UK initiative: QUEST Atmospheric Aerosols and Chemistry

Natural Emissions

- Produced through natural processes e.g. photosynthesis, respiration, wild fires etc.
- Often have a dependence on environmental factors
- Some of the most interesting “new” research topics deal with the feedbacks between climate and natural emissions.

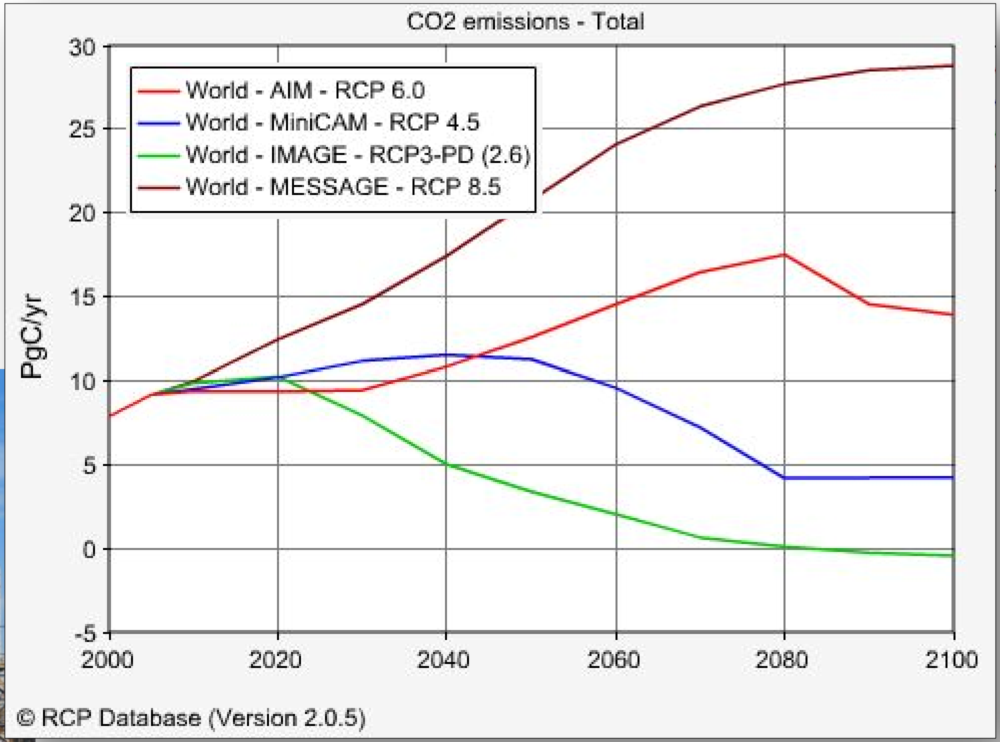




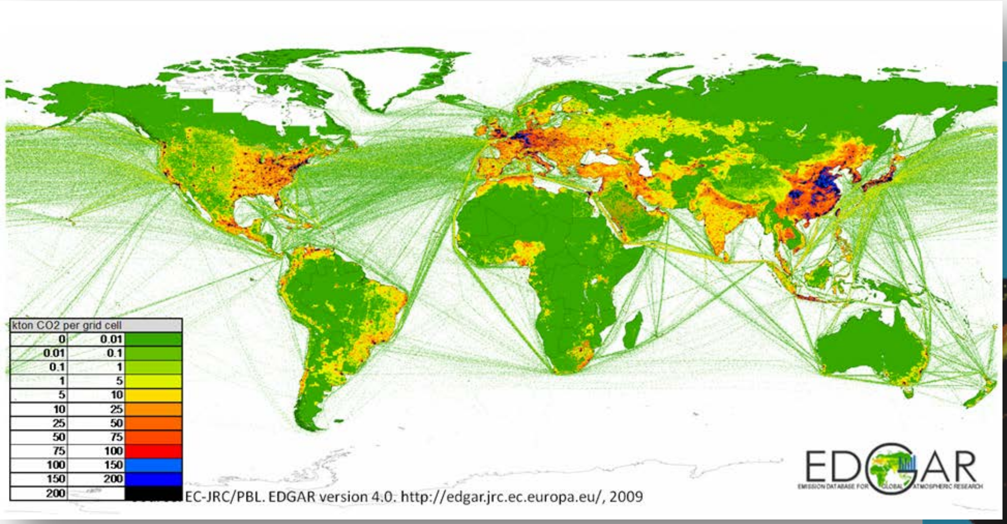
$$Flux_{HOI} = \left[O_{3(g)}\right] * \sqrt{\left[I^{-}{(aq)}\right]} * \left(\frac{3.56\times10^{5}}{ws} - 2.16\times10^{4}\right)$$

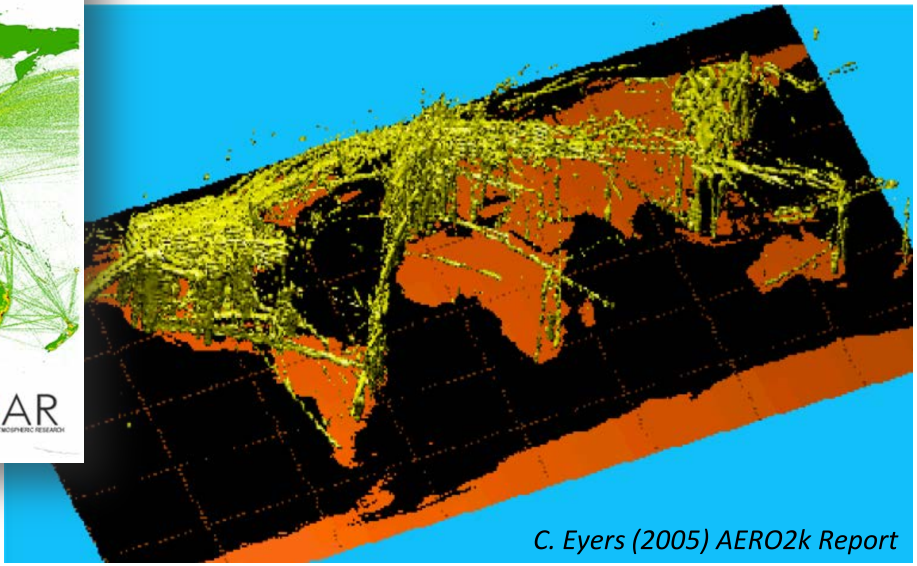
Anthropogenic Emissions

- Produced by man-made processes e.g. pasture burning, agriculture, industry etc. Can have "environmental dependence" but generally not.
- For some compounds anthropogenic emissions are the dominant source.
- Predicted to change due to socio-economic factors.



Compilation of Emissions Inventories



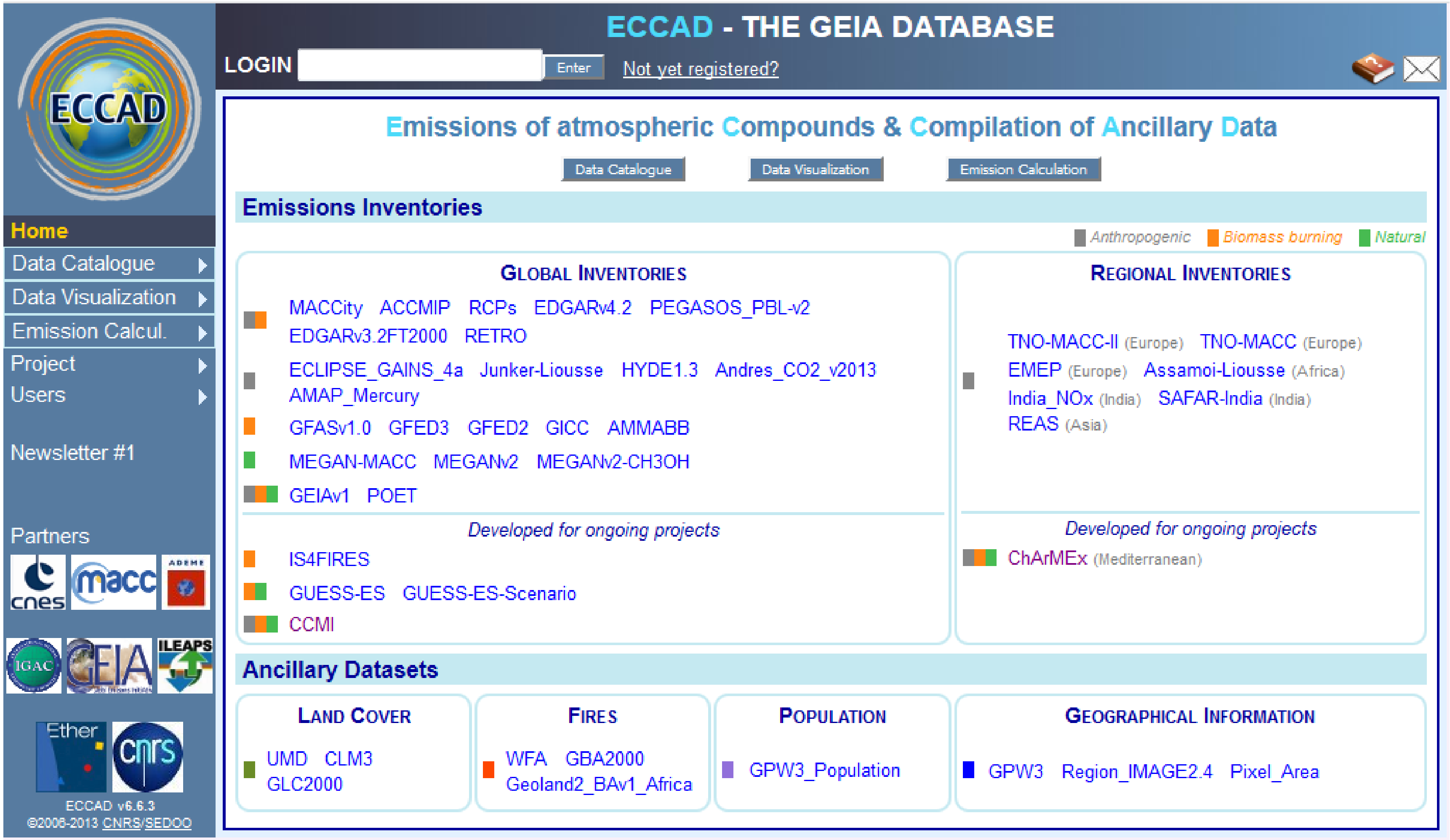


C. Eyers (2005) AERO2k Report

- Emissions data is typically provided in gridded inventories, either 2D or 3D depending on emission type.
- Global emission fluxes are often provided as monthly emissions fluxes (kg[species] m-2 s-1)
- Inventories are compiled with substantial effort using different techniques (e.g. top-down vs bottom-up)

Web Portals for Emissions Data

- GEIA Emissions Data Web Portal is a very good source of information for global emissions data http://eccad.sedoo.fr



Implementation of Emissions in Global Chemistry-Climate Models

- Choice of chemistry scheme determines the range of the emitted compounds.
- Emitted species can be "lumped" into compound groups.
- Online versus offline emissions.
- How to deal with sub-grid scale heterogeneity, plume processing (benefits versus computational expense).
- Temporal resolution: Monthly seasonal cycle versus diurnal/weekday cycle.
- Is emission height relevant? (e.g. aircraft emissions, biomass burning, explosive volcanic eruptions).

Sub-grid scale mixing of emissions in global models

- How realistic is the instantaneous dilution of regionally heterogeneous emissions in global model grid boxes?

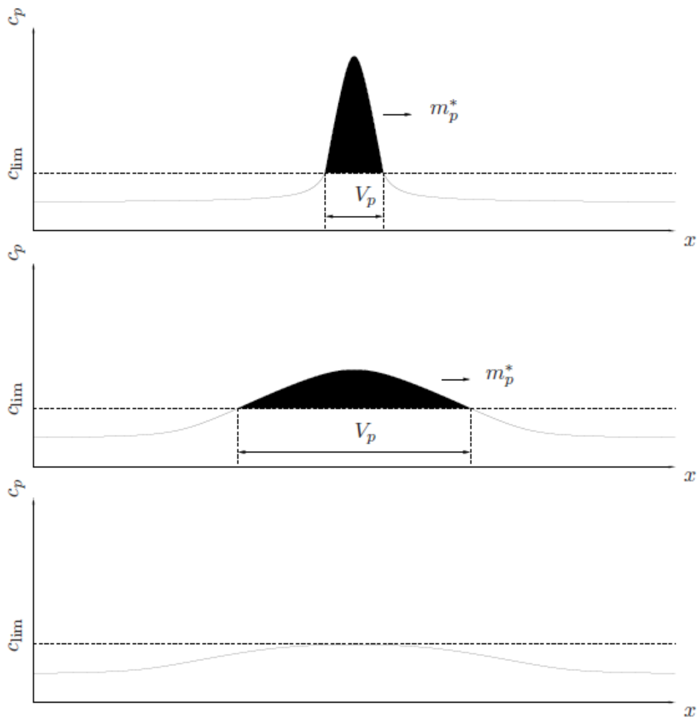


Fig. 6. Concept of plume lifetime used by Cariolle et al. (2009). Evolution of the excess of mass m_p^* over a threshold concentraion c_{lim} of a chemically conserved species in the plume, from $t = t_0$ (top panel) to $t = t_{lim}$ (bottom panel). The plume lifetime $t_p = t_{lim}$ is defined as the time when $m_p^* = 0$.

taken from Paoli et al., *GMD*, 2011

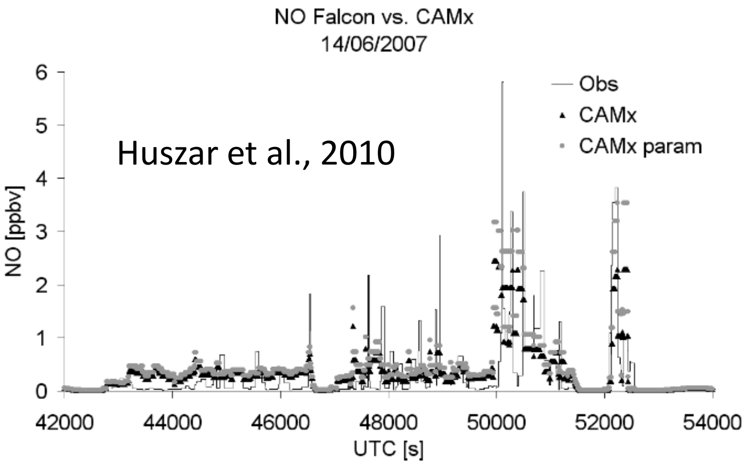


Fig. 14. Comparison of simulated nitrogen monoxide levels with aircraft ship emission measurements over the English Channel in June 2007. Black triangles denote the run without the ship plume parameterization, the gray circles the run with the parameterization.

Examples from the Literature (1)

Study by Huszar et al., 2010

Shipping NOx

Δ NOx due to plume model

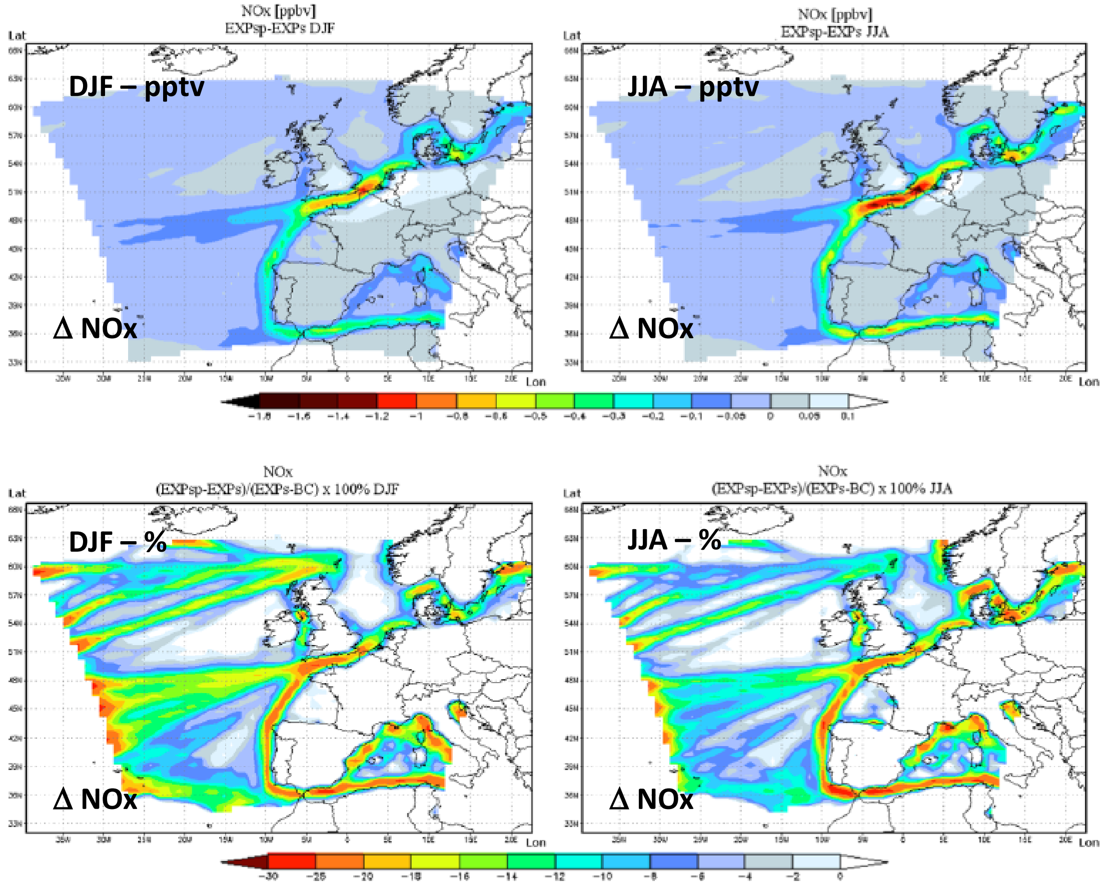
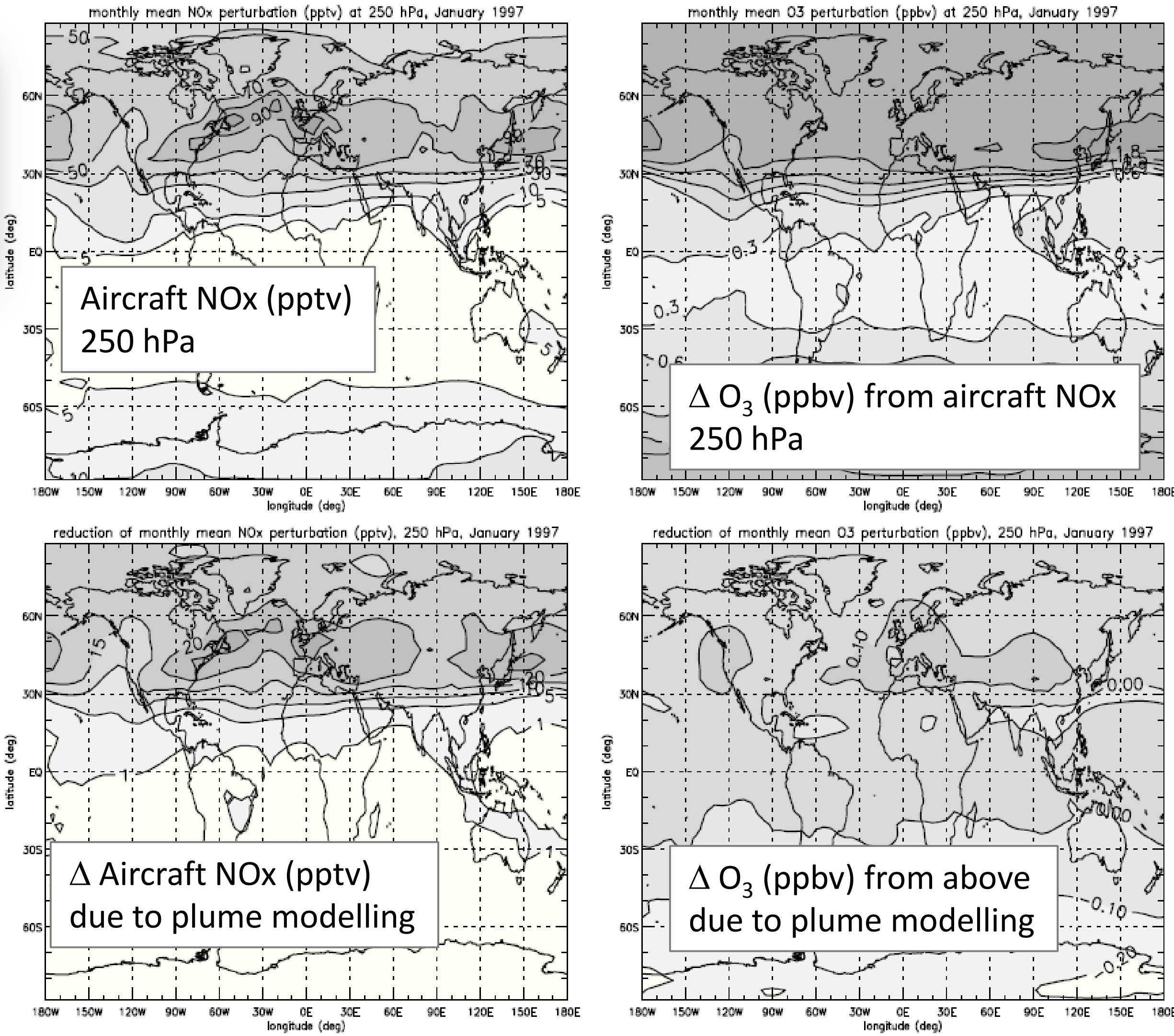


Fig. 23. Change in NO_x production by ship emissions. Top panels: difference of surface NO_x in experiments with and without plume model, ε_{NO_x} (Eq. 56) in ppbv for winter (left) and summer conditions (right). Bottom panels: same but for relative change $\varepsilon_{NO_{x\%}}$ (Eq. 57) (Huszar et al., 2010).

taken from Paoli et al., *GMD*, 2011

Examples from the Literature (2)

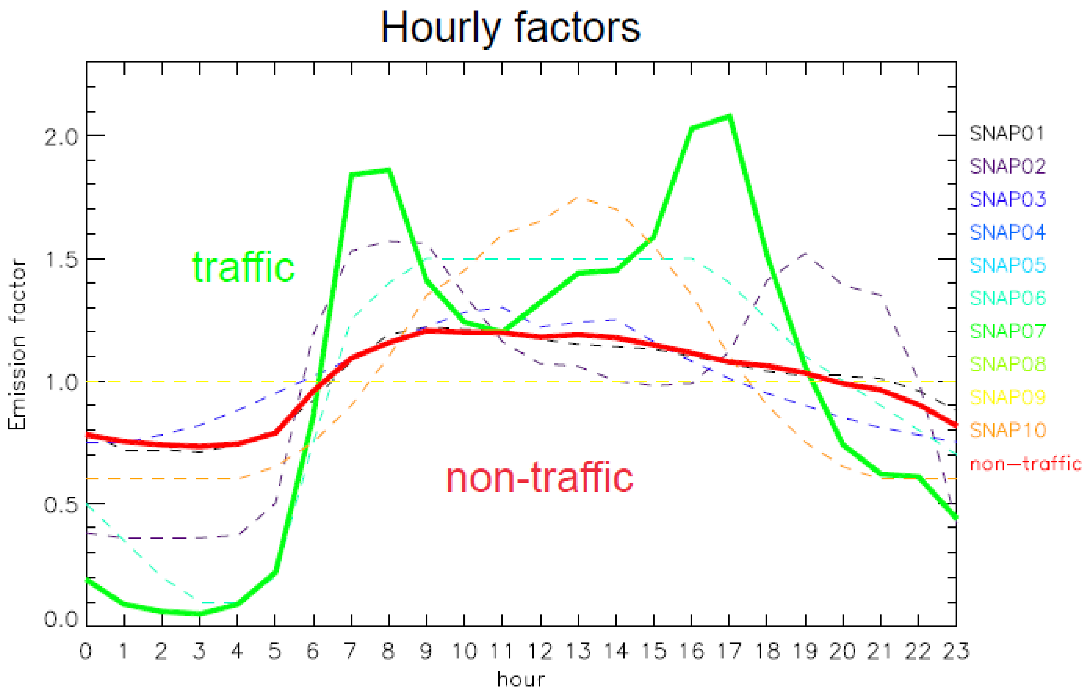
Study by Meijer et al., *JGR*, 2001



taken from Paoli et al., *GMD*, 2011

Temporal resolution of emissions data

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



Emissions in the UKCA Model

- Gas-phase emissions for StratTrop (CheST) chemistry

Emission Species	Units	Std trop	Trop-isop	RAQ chem	Strat chem	Strat+trop	Offline oxid
NOx Surface Emissions (treated as NO)		Y	Y	Y	Y	Y	
CH4 Surface Emissions		Y	Y	Y	Y	Y	
CO Surface Emissions		Y	Y	Y	Y	Y	
HCHO Surface Emissions		Y	Y	Y	Y	Y	
C2H6 Surface Emissions		Y	Y	Y		Y	
C3H8 Surface Emissions		Y	Y	Y		Y	
CH3COCH3 Surface Emissions		Y	Y	Y		Y	
CH3CHO Surface Emissions		Y	Y	Y		Y	
C5H8 (Isop) Surface Emiss			Y	Y		Y	
H2 Surface Emissions				Y*			
C4H10 Surface Emissions				Y			
C2H4 Surface Emissions				Y			
C3H6 Surface Emissions				Y			
Toluene Surface Emissions				Y			
o-xylene Surface Emissions				Y			
CH3OH Surface Emissions				Y			
NOx Aircraft Emissions (3D, treated as NO)		Y	Y	Y	Y	Y	

https://code.metoffice.gov.uk/doc/um/latest/umdp.html

taken from UMDP 084 vn10.9

Emissions in the UKCA Model

- Aerosol and Online Emissions

Emission Species	Units	Std trop	Trop-isop	RAQ chem	Strat chem	Strat+ trop	Offline oxid
If using Aerosol Chem							
Monoterpene Surface Emiss		Y	Y	Y		Y	Y
NVOC Surface Emiss (treated as CH3OH)			Y			Y	
SO2 Surface Emissions		Y	Y	Y	Y	Y	Y
DMS Surf Emiss (Land,ocean)		Y	Y	Y	Y	Y	Y
NH3 Surface Emissions		Y	Y	Y		Y	
SO2 High (Ind,forest,ship)		Y	Y	Y	Y	Y	Y
SO2 Volcanic Emissions (3D)		Y	Y		Y	Y	Y
for GLOMAP-mode (if using 5-mode setup)							
BC Fossil Fuel Emiss		Y	Y	Y		Y	Y
OC Fossil Fuel Emiss		Y	Y	Y		Y	Y
BC Biofuel Emissions		Y	Y	Y		Y	Y
OC Biofuel Emissions		Y	Y	Y		Y	Y
BC Biomass burn Emiss (3D or 2D)		Y	Y	Y		Y	Y
OC Biomass burn Emiss (3D or 2D)		Y	Y	Y		Y	Y
Online Emissions							
CH4 Wetland Emiss (in LSH - Optional)	μg(C)/m^2/s	Y	Y	Y	Y	Y	
Lightning NOx (treated as NO)	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	Y	Y
Primary marine OC (in GLOMAP-mode)	kg(POM)/m^2/s	Y	Y	Y	Y	Y	

https://code.metoffice.gov.uk/doc/um/latest/umdp.html

taken from UMDP 084 vn10.9

UKCA emissions use NetCDF format

- “New” emissions, using the NetCDF format, are no longer new and are now the standard method.
- NetCDF introduces flexibility and allows the use of different emission fields to account for independent source sectors for any given tracer.
- Metadata attributes in the NetCDF files avoid inconsistencies and allow cross-checking, e.g. of units, within the UKCA code.
- NetCDF files strive for CF compliance (but not always the case).
- Old ancillary file format only used for two files, DMS and chlorophyll, from oceanic sources (can be provided by ocean biogeochemistry model).

Attribute	Type	Variable	Mandatory
standard_name	char	emission	no
long_name	char	emission	yes if standard_name missing
tracer_name	char	emission	yes
units	char	emission	yes
hourly_scaling	char	emission	no
daily_scaling	char	emission	no
vertical_scaling	char	emission	no
lowest_level	int	emission	yes if vertical_scaling='high_level'
highest_level	int	emission	yes if vertical_scaling='high_level'
calendar	char	time coordinate	yes
calendar_flexible	int	time coordinate	no
update_freq_in_hours	int	global	yes
update_type	int	global	yes

taken from UMDP 084 vn10.9

NetCDF Attributes (1)

Information about how the emissions are to be implemented within UKCA is provided through meta data in the NetCDF files.

UKCA reads met data from NetCDF attributes.

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

- **update_type:** (follows same conventions as for ancillary files):
  - 0: Single time
  - 1: Time series
  - 2: Periodic time series

global attributes “**emission_type**” and “**update_type**” are often found together in earlier emissions files.
Both attributes do the same thing and **emission_type** will be discontinued!

NetCDF Attributes (2)

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

NetCDF Attributes (3)

- **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

Example emissions file

```
netcdf ukca_emiss_SO2_high {
dimensions:
        time = 732 ;
        model_level_number = 1 ;
        latitude = 144 ;
        longitude = 192 ;
        bnds = 2 ;
variables:
        float emissions_SO2_high(time, model_level_number, latitude, longitude) ;
                emissions_SO2_high:_FillValue = 1.e+20f ;
                emissions_SO2_high:standard_name = "tendency_of_atmosphere_mass_content_of_sulfur_dioxide_due_to_emission" ;
                emissions_SO2_high:long_name = "SO2 high level emissions" ;
                emissions_SO2_high:units = "kg m-2 s-1" ;
                emissions_SO2_high:highest_level = "8" ;
                emissions_SO2_high:lowest_level = "8" ;
                emissions_SO2_high:missing_value = 1.e+20 ;
                emissions_SO2_high:tracer_name = "SO2_high" ;
                emissions_SO2_high:um_stash_source = "m01s00i126" ;
                emissions_SO2_high:vertical_scaling = "high_level" ;
                emissions_SO2_high:cell_methods = "time: mean" ;
                emissions_SO2_high:grid_mapping = "latitude_longitude" ;
                emissions_SO2_high:coordinates = "forecast_period forecast_reference_time" ;
        int latitude_longitude ;
                latitude_longitude:grid_mapping_name = "latitude_longitude" ;
                latitude_longitude:longitude_of_prime_meridian = 0. ;
                latitude_longitude:earth_radius = 6371229. ;
        double time(time) ;
                time:axis = "T" ;
                time:units = "days since 1960-01-01 00:00:00" ;
                time:standard_name = "time" ;
                time:calendar = "360_day" ;
        int model_level_number(model_level_number) ;
                model_level_number:axis = "Z" ;
```

[.....]

```
// global attributes:
               :Conventions = "CF-1.5" ;
               :File_creation_date = "Thu Oct 12 11:48:57 2017" ;
               :File_version = "v2" ;
               :earth_ellipse = "Earth spheric model" ;
               :earth_radius = 6371229. ;
               :emission_type = "1" ;
               :global_total_emissions_2000 = "66.572 Tg SO2 per year" ;
               :grid = "regular 1.875 x 1.25 degree longitude-latitude grid (N96e)" ;
               :history = "Thu Oct 12 11:48:57 2017: regrid_SO2_high_emissions_n96e_360d.py \n",
                       "combine_all_sources_SO2_high_1960-2020.pro" ;
               :institution = "Centre for Atmospheric Science, Department of Chemistry, University of Cambridge, U.K." ;
               :molecular_weight = 64.07f ;
               :molecular_weight_units = "g mol-1" ;
               :reference = "Granier et al., Clim. Change, 2011; Lamarque et al., Atmos. Chem. Phys., 2010" ;
               :source = "combined_sources_SO2_high_1960-2020_greg.nc" ;
               :title = "Time-varying monthly surface emissions of sulfur dioxide from 1960 to 2020 (from selected anthropogenic source sectors only)" ;
               :um_version = "10.6" ;
               :update_freq_in_hours = "120" ;
               :update_type = "1" ;
data:
```

Implementation of time-varying emissions

- Time-varying emissions for the ACSIS Project:
  http://www.ukca.ac.uk/wiki/index.php/Emissions_for_ACSIS

- Typically compilation of sector data from **various sources** necessary
- **Lumping** of VOC groups into emitted compounds is required
- Choices required regarding **calendar setting** (360-day vs Gregorian):
  Consistency w.r.t. to annual emitted totals or w.r.t. monthly emissions flux?
- Generation of the model's emissions files requires **mass-conserving regridding** (i.e. no interpolation!) of the raw data to the model grid, in order to conserve the mass fluxes.

Tabular Overview of the ACSIS Emissions

The table below gives a concise overview of what data sources have been lumped into the individual emissions files. A more detailed description of the emissions is shown in the following sections on this page.

#	Emissions File	UKCA Tracer	Total Emissions Year 1960	Total Emissions Year 2000	Sources	Sector Contributions Year 2000	Source Data Files	Timeseries Data
1	ukca_emiss_NO.nc	NO	53.0 Tg NO	90.7 Tg NO	anthropogenic	69 Tg NO	MACCity_anthro_NOx_1960-2020_14412.nc	NOx.zip
					biomass burning	10 Tg NO	**1960–2008:** accmip_maccity_emissions_historic_NOx_biomassburning_YEAR_0.5x0.5.nc **2009–2020:** accmip_interpolated_emissions_RCP85_NOx_biomassburning_YEAR_0.5x0.5.nc	
					soil	12 Tg NO (scaled)	nox_soil_0.5_0.5.nc	
2	ukca_emiss_NO_aircrft.nc	NO	0.398 Tg NO	1.82 Tg NO	anthropogenic	1.82 Tg NO	MACCity_anthro_NOx_aviation_1960-2010_57144.nc	NOx_aircrft.zip
3	ukca_emiss_CO.nc	CO	850.5 Tg CO	1068 Tg CO	anthropogenic	611 Tg CO	MACCity_anthro_CO_1960-2020_12697.nc	CO.zip
					biomass burning	349 Tg CO	**1960–2008:** accmip_maccity_emissions_historic_CO_biomassburning_YEAR_0.5x0.5.nc **2009–2020:** accmip_interpolated_emissions_RCP85_CO_biomassburning_YEAR_0.5x0.5.nc	
					biogenic	89 Tg CO	MEGAN-MACC_biogenic_CO_1980-2010_66468.nc	
					oceanic	20 Tg CO	POET_oceanic_CO_1990_84299.nc	
4	ukca_emiss_CH4.nc	CH4	(not used)				(climatological boundary condition)	
					anthropogenic	3.3 Tg C2H6 7.7 Tg C2H4 3.3 Tg C2H2 Total: 15.4 Tg lumped C2H6	MACCity_anthro_ethane_1960-2020_98245.nc MACCity_anthro_ethene_1960-2020_98274.nc accmip_interpolated_emissions_historic/RCP85_ethyne_anthropogenic_YEAR_0.5x0.5.nc accmip_interpolated_emissions_historic/RCP85_ethyne_ships_YEAR_0.5x0.5.nc	
					biomass	2.3 Tg C2H6 4.8 Tg C2H4	**1960–2008:** accmip_maccity_emissions_historic_ethane_biomassburning_YEAR_0.5x0.5.nc accmip_maccity_emissions_historic_ethene_biomassburning_YEAR_0.5x0.5.nc accmip_maccity_emissions_historic_ethyne_biomassburning_YEAR_0.5x0.5.nc	

Summary

- Numerical models use **inputs** (e.g. emissions), operate on these and produce **outputs (results)**. **Quality of these inputs is essential** in atmospheric chemistry modelling as they stand at the beginning of the chemical processes.
- A combination of **anthropogenic and natural emissions data** is required to represent atmospheric chemistry in global models. **Choice of** emitted **compounds** and their **implementation** depends highly on the **objective of the study**. There is more than one correct way how emissions data can be included in models (and there are even more incorrect ways!).
- UKCA uses input data files in NetCDF format which allows for **consistency checking and flexibility** in the way how the emissions are released in the model (altitude, temporal frequency, source sectors etc.)
- A concise description of the UKCA emissions implementation is available in **UMDP 84 (UKCA) Chapter 10**.