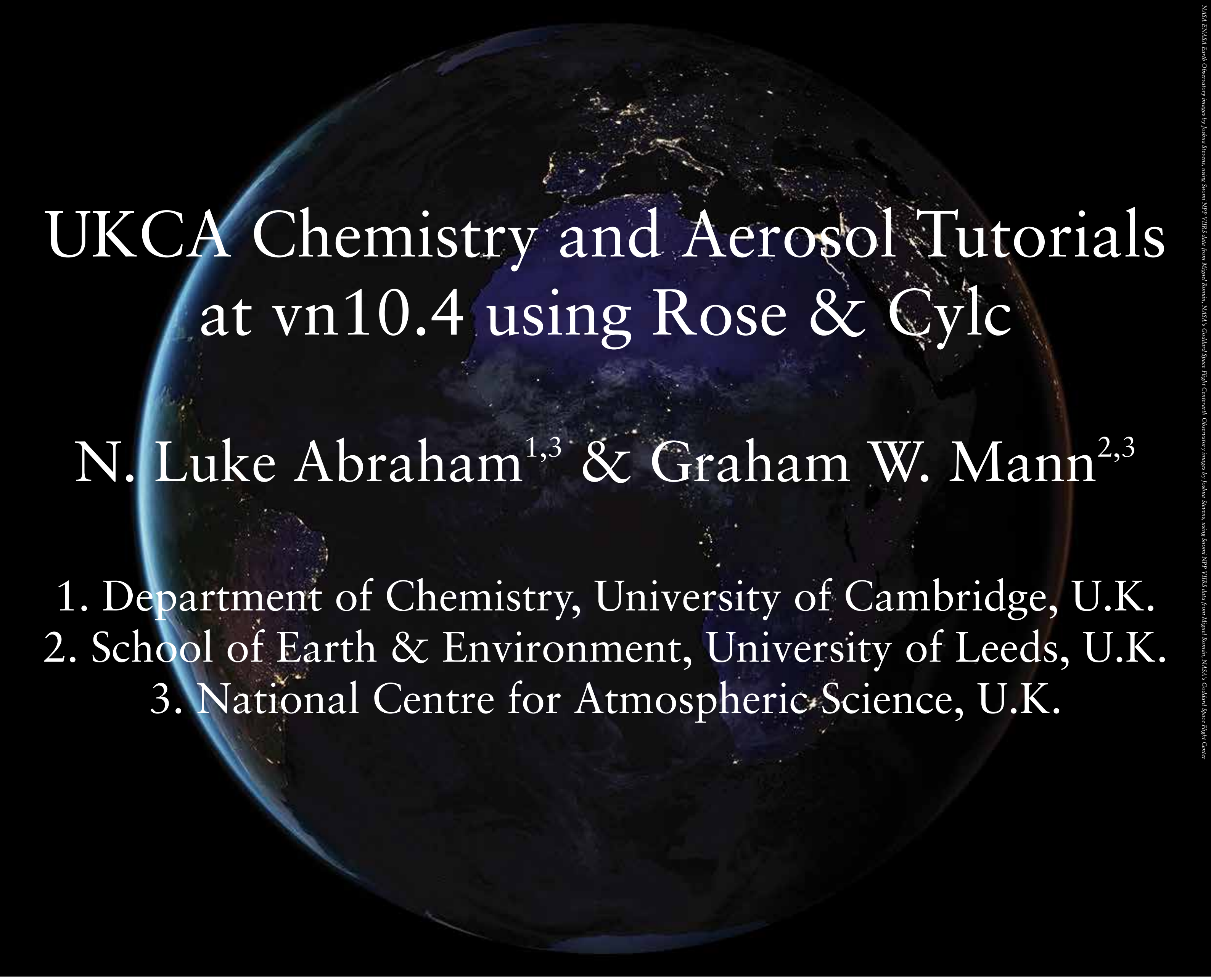

UKCA Chemistry and Aerosol Tutorials at vn10.4 using Rose & Cylc

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NASA ENASA Earth Observatory images by Joshua Stevens, using Suomi NPP VIIRS data from Miguel Román, NASA's Goddard Space Flight Centerarth Observatory images by Joshua Stevens, using Suomi NPP VIIRS data from Miguel Román, NASA's Goddard Space Flight Center

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September 2016

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UKCA Chemistry and Aerosol Tutorials at vn10.4

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4 using Rose & Cylc

The following tutorials will teach you how to use various aspects of UKCA, and the parts of Rose (the Unified Model's python-based user interface) that are specific to UKCA.

- ### Things to know before you start

General use of the Rose and UKCA:

1. Running existing UKCA Suite
2. Exploring Rose
3. What is STASH?
4. Adding new chemical tracers
5. Adding new emissions
6. Adding new chemical reactions
7. Adding dry deposition of chemical species
8. Adding wet deposition of chemical species
9. Adding new UKCA chemical diagnostics
10. Examining Aerosol Optical Depth changes
11. Changing the aerosol configuration
12. Diagnosing the radiative effect of aerosols

The slides from the Workshop run in January 2017 can be found here: UKCA Tutorial Slides (1-9) (//www.ukca.ac.uk/wiki/index.php/File:2017_NLA_UKCA_Tutorial_01-09.pdf)

These tutorials are an update and expansion of the tutorials which were at UM8.2 and UM8.4.

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ACITES ATMOSPHERIC CHEMISTRY IN THE EARTH SYSTEM

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol Tutorials: Things to know before you start the vn10.4 practicals

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

You will need to have the details of your PUMA and ARCHER accounts to hand.

Contents

Before you begin the UKCA Tutorials

These tutorials assume that you are familiar with FCM, and training on this can be found here:

http://cms.ncas.ac.uk/wiki/Fcm

The UM FCM tutorial that is linked from this page uses the old user interface (the *"UMUI"*), so will be less relevant here.

You should also familiarise yourself with Rose & Cylc, and more information on these can be found here:

http://cms.ncas.ac.uk/wiki/RoseCylc

The Met Office provide some on-line UM specific Rose training here:

https://code.metoffice.gov.uk/doc/um/latest/um-training/index.html

Also, if you do not have a PUMA or ARCHER account, you can use the Met Office provided Virtual Machine to run the VM. You should follow the instructions here (you will need the Ubuntu 15.10 image with 3GB of RAM)

https://github.com/metomi/metomi-vms

before following the instructions here to get the UM working.

https://code.metoffice.gov.uk/trac/um/wiki/VirtualMachine

It will soon be possible to run a simple UKCA suite in the VM, but this requires at least 6GB of RAM to run successfully.

Accounts

To run these tutorials the minimum you will need is

- an account on the Met Office Science Repository Service (https://code.metoffice.gov.uk)

which will then allow you to run the tutorials in a Virtual Machine (**coming soon**) (https://code.metoffice.gov.uk/trac/um/wiki/VirtualMachine) .

To run these on ARCHER you will need

- a PUMA account
- an ARCHER account

For information on how to get these, please see the Getting Started with UKCA page.

Developing code for the UM

During this tutorial you will be creating tickets on the Met Office Science Repository Service (https://code.metoffice.gov.uk) , and making code changes to UM branches. Please note that **this is a *live* system**, used by scientists all over the world to develop their code. However, **please don't worry about breaking anything**, as there are practices in place to prevent this.

For more information about developing for the UM, please see the Working Practices for UM Development with Rose, FCM and trac (https://code.metoffice.gov.uk/trac/um/wiki/working_practices) .

UKCA Training Suite

To set-up using the UM with Rose & Cylc correctly, go to

- http://cms.ncas.ac.uk/documents/training/November2016/UM_practicals/getting-setup.html

and follow the instructions from **Section 2.2** onwards if you are using Linux/Mac (after opening a terminal).

Note: when entering MOSRS password, a rose window will open behind everything all your other windows. You will also need to enter your username here to complete the process.

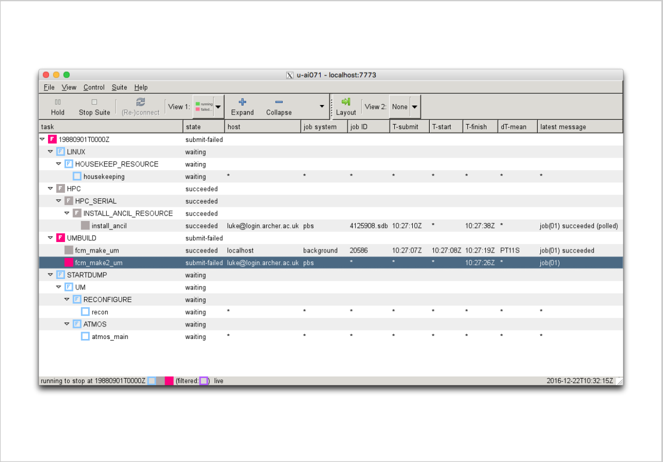
When you have completed this, you should launch the Rose browser by typing

```
rosie go &
```

and there you should search for suite **u-ai071** and make a copy of it.

When you have copied the suite, you will need to remember to change the username & tic code in *suite conf* → *Machine Options*.

Manual Compiling

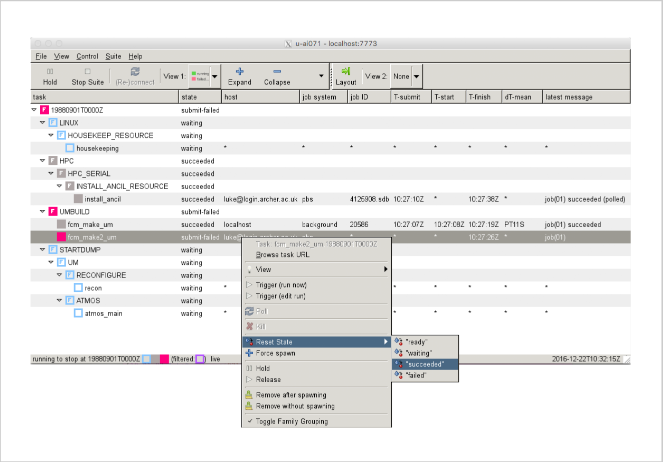


u-ai071 - localhost:7773

task	state	host	job system	job ID	T-submit	T-start	T-finish	dT-mean	latest message
19880901T0000Z	submit-failed								
LINUX	waiting								
HOUSEKEEP_RESOURCE	waiting								
housekeeping	waiting	*	*	*	*	*	*	*	*
HPC	succeeded								
HPC_SERIAL	succeeded								
INSTALL_ANCIL_RESOURCE	succeeded								
install_ancil	succeeded	luke@login.archer.ac.uk	pbs	4125908.sdb	10:27:10Z	*	10:27:38Z	*	job(01) succeeded (polled)
UMBUILD	submit-failed								
fcm_make_um	succeeded	localhost	background	20586	10:27:07Z	10:27:08Z	10:27:19Z	PT11S	job(01) succeeded
fcm_make2_um	submit-failed	luke@login.archer.ac.uk	pbs	*	*	*	10:27:26Z	*	job(01)
STARTDUMP	waiting								
UM	waiting								
RECONFIGURE	waiting								
recon	waiting	*	*	*	*	*	*	*	*
ATMOS	waiting								
atmos_main	waiting	*	*	*	*	*	*	*	*

running to stop at 19880901T0000Z (filtered:) live 2016-12-22T10:32:15Z

Gcylc window showing the fcm_make2_um task in the submit-failed state



u-ai071 - localhost:7773

task	state	host	job system	job ID	T-submit	T-start	T-finish	dT-mean	latest message
19880901T0000Z	submit-failed								
LINUX	waiting								
HOUSEKEEP_RESOURCE	waiting								
housekeeping	waiting	*	*	*	*	*	*	*	*
HPC	succeeded								
HPC_SERIAL	succeeded								
INSTALL_ANCIL_RESOURCE	succeeded								
install_ancil	succeeded	luke@login.archer.ac.uk	pbs	4125908.sdb	10:27:10Z	*	10:27:38Z	*	job(01) succeeded (polled)
UMBUILD	submit-failed								
fcm_make_um	succeeded	localhost	background	20586	10:27:07Z	10:27:08Z	10:27:19Z	PT11S	job(01) succeeded
fcm_make2_um	submit-failed	luke@			*	*	10:27:26Z	*	job(01)
STARTDUMP	waiting								
UM	waiting								
RECONFIGURE	waiting								
recon	waiting	*			*	*	*	*	*
ATMOS	waiting								
atmos_main	waiting	*			*	*	*	*	*

running to stop at 19880901T0000Z (filtered:) live 2016-12-22T10:32:15Z

Resetting the state of the fcm_make2_um task

The UKCA Training Suite has been altered slightly to allow it to be easily manually compiled. This can be selected as an option in **suite conf** → **Machine Options**. With this set to **true**, when the suite runs the ***fcm_make2_um*** task will enter the ***submit-failed*** state. Then, on **ARCHER**, you should then change directory into

```
$HOME/cylc-run/[SUITE-ID]/log/job/19880901T0000Z/fcm_make2_um/NN
```

and compile the `um-atmos` and `um-recon` executables by typing

```
./job
```

This will take around 7-12 minutes to compile. You can follow the progress of this process in detail by `tail`-ing the following file

```
$HOME/cylc-run/[SUITE-ID]/share/fcm_make_um/fcm-make2.log
```

Once this step has completed, you can send the rest of the suite off by going back to the Gcylc window and **right-clicking on the *fcm_make2_um*** task and click **Reset State** → **"succeeded"**. This will then allow the rest of the tasks to start in sequence.

Note: manually compiling in this way means that you will no longer have the *job.out* or *job.err* files. You should instead look in the *fcm-make2.log* file.

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- This page was last modified on 7 January 2017, at 00:03.

UKCA Chemistry and Aerosol vn10.4 Tutorial 1

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Before starting these tutorials you should first make sure that you have completed the setup instructions (http://cms.ncas.ac.uk/documents/training/November2016/UM_practicals/getting-setup.html) . If you are using Linux or macOS you will only need to complete section 2.2 onwards.

Copying and Running an Existing Rose Suite

You will need to login to PUMA, e.g.

```
ssh -Y username@puma.nerc.ac.uk
```

You should then be asked for the SRS password.

Then launch the UM graphical user interface by:

```
rosie go
```

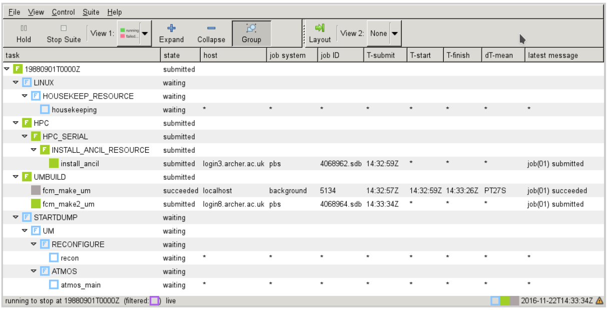
This should then load up a blank interface. Go to **Edit** ⟶ **Data source** and select **u**. The go to the search panel and type **u-ai071** and press return. This will then show all the suites that have u-ai071 in it's history or title. You should just select suite u-ai071 and not any of the others.

Right-click on suite u-ai071 and click **copy suite**. A new box will open asking for the project - it is fine to press **Forward** here. On the next panel, it's fine to just press **OK** again as well.

The suite will now copy and checkout to your `/home/$USER/roses` directory, and will also appear when running `rosie go`.

You should now right-click ⟶ edit (or double-click) on this new suite, and click **run**, which is symbolised by a *play* symbol (i.e., a large grey arrow-head pointing to the right).

This suite has been configured to **manually compile**, so you should follow the instructions on how to do that, to be sure that you can compile your suite as quickly as possible. It will take about 10 minutes to compile the code, followed by about 90 seconds to run the reconfiguration step, and then 7 minutes to run the UM itself.



task	state	host	job system	job ID	T-submit	T-start	T-finish	dT-mean	latest message
19880901T0000Z	submitted								
LINUX	waiting								
HOUSEKEEP_RESOURCE	waiting								
housekeeping	waiting	*	*	*	*	*	*	*	*
HPC	submitted								
HPC_SERIAL	submitted								
INSTALL_ANCIL_RESOURCE	submitted								
install_ancil	submitted	login3.archer.ac.uk	pbs	4068962.sdb	14:32:59Z	*	*	*	job(01) submitted
UMBUILD	submitted								
fcm_make_um	succeeded	localhost	background	5134	14:32:57Z	14:32:59Z	14:33:26Z	PT27S	job(01) succeeded
fcm_make2_um	submitted	login8.archer.ac.uk	pbs	4068964.sdb	14:33:34Z	*	*	*	job(01) submitted
STARTDUMP	waiting								
UM	waiting								
RECONFIGURE	waiting								
recon	waiting	*	*	*	*	*	*	*	*
ATMOS	waiting								
atmos_main	waiting	*	*	*	*	*	*	*	*

running to stop at 19880901T0000Z (filtered:) live 2016-11-22T14:33:34Z

Figure 1: GCylc running.

Version Control

Rose suites are all held under version control, using fcm (http://cms.ncas.ac.uk/wiki/Fcm) . When making changes to a suite, you will need to **save** it before you can **run** the suite. Once you are happy with the settings, you can also **commit** these changes back to the repository - to do this change directory to the

```
/home/$USER/roses/[SUITE-ID]
```

and then type

```
fcm commit
```

a text editor will then open, and you should type a short message describing what the changes you have made do. You should then close the editor and type **y** in the terminal. It is recommended that you commit frequently (even on configurations that aren't working) as this protects you against mistakes and accidental deletions etc.

These suites can be viewed on the SRS here: https://code.metoffice.gov.uk/trac/roses-u (password required) (https://code.metoffice.gov.uk/trac/roses-u)

Output Directory Structure

The output directory structure of rose suites are rather complex:

- You can find the latest & full *job.out* files in

  `/work/n02/n02/$USER/cylc-run/[SUITE-ID]/log/job/YYYYMMDDTttttZ/[JOB NAME]/NN`

  e.g. /work/n02/n02/luke/cylc-run/u-ag308/log/job/19880901T0000Z/atmos/NN

  This file contains what the UM writes out using the `umPrint` subroutine (what used to be written out using `WRITE(6)` statements).

- Output from the individual processors (which are updated as the job is running can be found in

  `/work/n02/n02/$USER/cylc-run/[SUITE-ID]/work/YYYYMMDDTttttZ/[JOB NAME]/pe_output`

  e.g. /work/n02/n02/luke/cylc-run/u-ag308/work/19880901T0000Z/recon/pe_output

  A handy command to check the progress of the job is

  ```
  tail -1000f [SHORT SUITE-ID].fort6.pe00 | grep Atm_Step
  ```

- Output files in 64-bit fieldsfile format can be found (on ARCHER) in

  `/work/n02/n02/`**`$USER`**`/cylc-run/`**`[SUITE-ID]`**`/share/data/History_Data`
  Files often have the following naming convention

  `[SHORT SUITE-ID]``a.p`**`[abcdefghijkmsyx]`**`YYYYMMDD`

  e.g. `ag308a.pk19880901`

Whilst this suite is running, take a look at Tutorial 2: Exploring Rose.

Tutorial 2

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 2

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

Exploring Rose

If you are familiar with the UMUI, you will see that Rose is quite different. As well as a complete re-write of the user interface, a lot of the namelists have been streamlined and also other things, such as how STASHmaster files are read (for user diagnostics etc.), have also been changed.

Take a look at your suite, and click through the options. There are 2 key sections that you will need to consider:

fcm_make_um

This section controls which fcm branches are used by the model, and also what compiler settings are used etc. You should go to **fcm_make_um** ⟶ **env** ⟶ **Sources** to see what branches are being used. During the course of these tutorials you will make a branch and add it here to complete the tutorial tasks. You can add both relative paths to the repository (starting with `branches/`) and absolute paths to a working copy (starting with `/home/`).

um

Click the arrow by **um** to view the list of sections. We'll be most interested in the **namelist** section, which contains all the settings that configure the science that will be done in this configuration of the UM, including the UKCA-specific options, and also when adding more output. We will mostly be concerned with 2 sections:

STASH Requests

Go to **um** ⟶ **namelist** ⟶ **Model Input and Output** ⟶ **STASH Requests and Profiles** ⟶ **STASH Requests** to view all the model output that has been requested by this suite. This list can be quite extensive, and we will cover adding more output in Tutorial 3: What is STASH?. During these tutorials this will be know as **the STASH panel**.

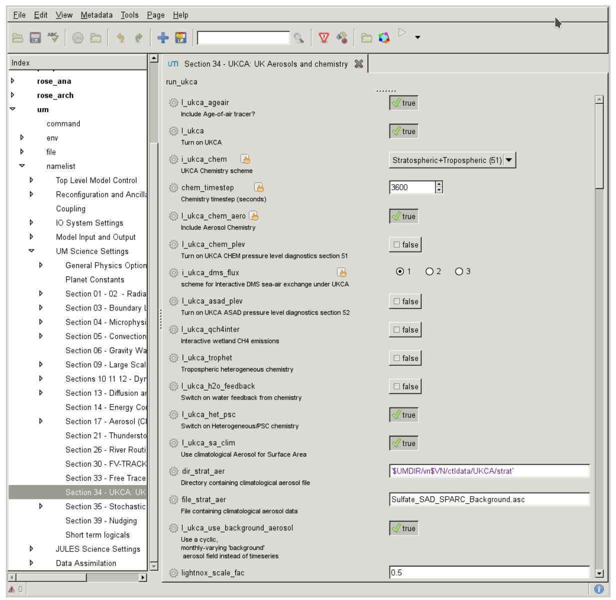
Section 34 - UKCA: UK Aerosols and Chemistry

Go to **um** ⟶ **namelist** ⟶ **UM Science Settings**. This contains all the different science sections, and by clicking on each panel you can see the settings for each. If you click on **Section 34 - UKCA: UK Aerosols and Chemistry** you will be able to see the UKCA settings. During these tutorials this will be known as **the UKCA panel**.

In Rose there is a 1:1 correspondence between the name of the variable in Rose, and the name of the variable in the namelist and hence the UM. This means that it can be easy to find what variable you might be interested in by first finding the appropriate variable in Rose (e.g. l_ukca_ageair). By the name of each variable is a cog - if you click this you can view **info** about the variable, which lists all the information the Rose has been given about it, e.g.

```
Data
name  l_ukca_ageair
value  .true.
comments
error
flags
ignored_reason
warning

Metadata
compulsory  true
description  Include Age-of-air tracer?
fail-if  namelist:run_ukca=i_ukca_chem==0 and this=='.false.'
full_ns  /um/namelist/UM Science Settings/section34
help  Allows the Age-of-Air tracer to be included
in the model configuration.
id  namelist:run_ukca=l_ukca_ageair
sort-key  a09
type  logical
```



Section 34 - UKCA: UK Aerosols and chemistry

run_ukca

l_ukca_ageair ☑ true
Include Age-of-air tracer?

l_ukca ☑ true
Turn on UKCA

i_ukca_chem Stratospheric+Tropospheric (51)
UKCA Chemistry scheme

chem_timestep 3600
Chemistry timestep (seconds)

l_ukca_chem_aero ☑ true
Include Aerosol Chemistry

l_ukca_chem_plev □ false
Turn on UKCA CHEM pressure level diagnostics section 51

i_ukca_dms_flux ● 1 ○ 2 ○ 3
scheme for Interactive DMS sea-air exchange under UKCA

l_ukca_asad_plev □ false
Turn on UKCA ASAD pressure level diagnostics section 52

l_ukca_qch4inter □ false
Interactive wetland CH4 emissions

l_ukca_trophet □ false
Tropospheric heterogeneous chemistry

l_ukca_h2o_feedback □ false
Switch on water feedback from chemistry

l_ukca_het_psc ☑ true
Switch on Heterogeneous/PSC chemistry

l_ukca_sa_clim ☑ true
Use climatological Aerosol for Surface Area

dir_strat_aer '$UMDIR/vn$VN/ctldata/UKCA/strat'
Directory containing climatological aerosol file

file_strat_aer Sulfate_SAD_SPARC_Background.asc
File containing climatological aerosol data

l_ukca_use_background_aerosol ☑ true
Use a cyclic,
monthly-varying 'background'
aerosol field instead of timeseries

lightnox_scale_fac 0.5

Figure 1: The UKCA panel in Rose.

You can also click **help**, which lists the help text associated with each variable. If you are not sure about a variable, looking at the info can be very informative. Due to the way the change process of the UM works, all variables must have information, such as the above, supplied, and any new science that has been added also needs to be added to each sections documentation paper.

search

Unlike the UMUI, there is a search bar in rose. It works best if you know the name of a variable, although it is still very useful to find options if you're not sure where they are.

Please take some time to browse through the rose suite, and get a feel for where things are. If you previously used the UMUI, you might want to try to locate comparable panels to see how things have changed.

Tutorial 3

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 3

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

When using the UM, it is likely that you will want to add new diagnostics, and we will cover writing out chemical fluxes in a later tutorial. Here we will cover selecting new diagnostics in STASH.

Contents

Task 3.1: add new output

TASK 3.1: Output the daily-mean UKCA ozone (section 34 item 001) field to the **UPK** output stream, and then add-in the equivalent diagnostic on pressure levels using the DP36CCM domain.

Hint	[hide]
You will need to remember to run the TidyStashTransform macro once you have added the diagnostics in the STASH panel. You will need to output the Heavyside function from the pressure-level diagnostics section, otherwise you will get an error. You will need to set the `l_ukca_chem_plev` logical to **true**.	

In the following page you will learn more about how the Unified Model's output is organised and managed. You should use this information to complete the task above. A worked solution is provided at the end of the tutorial.

What is STASH?

STASH is the Unified Model's storage handling and diagnostic system. It is designed to cope with the many different configurations that the UM can be used in, but still provide output in a consistent and standard way. A full technical description of STASH can be found in **Unified Model Documentation Paper C4** which can be downloaded from the Met Office Science Repository Service (password required) (https://code.metoffice.gov.uk/doc/um/latest/umdp.html) .

Prognostic and Diagnostic Fields

The UM considers variables (or *fields*) to be of two different types, *prognostic* or *diagnostic.* **Prognostic** fields are ones which the model must have values for, prior to each timestep, as e.g. the equations of motion the model solves require these fields (these are fields such as specific humidity or potential temperature), so they must exist in the model start dump. **Diagnostic** fields are all other fields that are derived from prognostic ones, and as such the model does not need to have prior values for these. Ancillary files (such as emissions, SSTs etc) contain prognostic fields. UKCA requires around 137 prognostic fields in the GA7+StratTrop configuration, and could in theory provide almost 2000 diagnostic fields on model levels, many of which have pressure-level equivalents.

From a user's perspective, STASH is used to output fields during the run, and from this point of view it does not matter if these are prognostic or diagnostic fields. However, you will need to consider these differences when you add new chemical tracers.

STASH Sections and Items

Each field that is considered by STASH has a unique address which is given by a **section** and an **item** number. Prognostic fields are mostly held in section 0 (with the exception of tracers) and diagnostics are organised by areas of the code, e.g. short-wave radiation diagnostics are held in section 1, long-wave radiation diagnostics are held in section 2 etc. Some sections will always be on, and some sections will only be on if a certain process is selected, e.g. the interactive land-surface scheme. Each section can hold up to 999 items, where each item is a separate prognostic or diagnostic field, and can be either 2D or 3D.

Each field has its own entry in a **STASHmaster file**. There is a master list of fields which is held in the *STASHmaster_A* file, a copy of which is located in each branch at

```
rose-meta/um-atmos/vnX.Y/etc/stash/STASHmaster/STASHmaster_A
```

If you make changes to this, to add your own diagnostics, you will need to make changes to the

```
rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A
```

file, and then change where Rose looks for the **metadata** associated with your suite. This will be covered in more detail when you add new chemical tracers.

The term *HEAD* here refers to the "head" of the branch. For any new branch at a particular model version (e.g. vn10.6) the STASHmaster_A file in *HEAD* and e.g. *vn10.6* will (initially) be the same.

STASH Panel

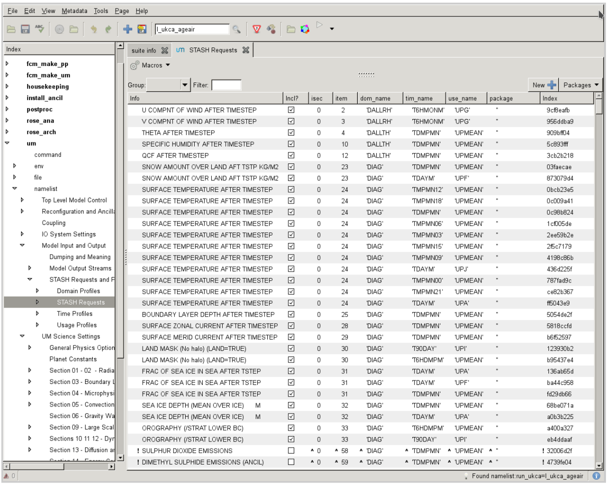
The STASH panel can be found at **um** ⟶ **namelist** ⟶ **Model Input and Output** ⟶ **STASH Requests and Profiles** ⟶ **STASH Requests**.

It is usually intially sorted by section/item numbers, but you can change the ordering by clicking on the items on the bar at the top (e.g. **use_name**). This can be helpful to see which items are going to which output stream.

To add new output, click the **New** button (with the large plus symbol on it), and this will open the *Add new STASH requests panel*. This lists all the available STASH output by section. You can scroll down to the section you want, click the small arrow on the left, scroll down to the diagnostic that you want and either right-click on it and click **Add STASH request**, or select it and then click the **Add** button in the top right-hand corner of the panel.

Once this has been added to the main STASH panel, you will get a message, similar to **Added request as namelist: streq(1)**. You will also find that a red warning triangle has appeared in the rose editor. This will disappear once you fill-in the *dom_name*, *tim_name*, and *use_name* entries for it. This can be done by clicking next to the red X that is in each column and selecting the correct value from the drop-down menu.

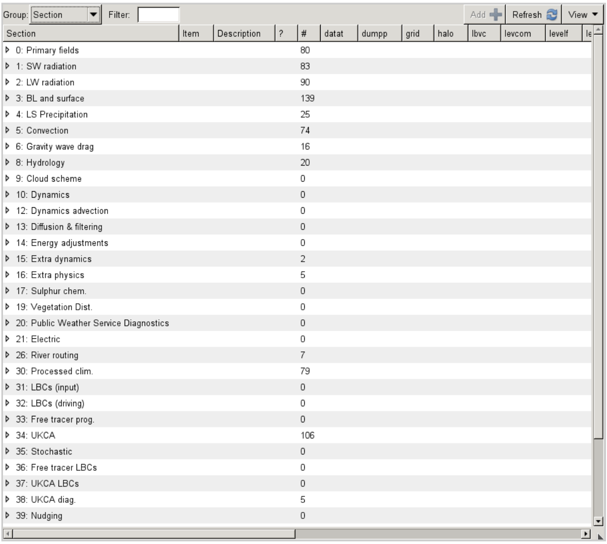
Once you have selected entries for each usage field, you will need to run the **TidyStashTransform** macro. When the STASH entry was created it was given the the namelist value *streq(1)*. This is a default value, and the correct namelist index needs to be generated for each STASH item (each is unique to the choices made, which also prevents duplicate entries being created). To do this, click the **Macros** drop-down menu from the top-left of the panel and select the **stashindices.TidyStashTransform** option. This will process the STASH requests, and any entries where the index doesn't match will be listed. Click **OK**, and this will then apply the correct index to the request, which will be a string of seemingly-random letters and numbers.



Info	Incl?	isec	item	dom_name	tim_name	use_name	package	Index
U COMPNT OF WIND AFTER TIMESTEP	☑	0	2	'DALLRH'	'T6HMONM'	'UPG'	''	9cf8eafb
V COMPNT OF WIND AFTER TIMESTEP	☑	0	3	'DALLRH'	'T6HMONM'	'UPG'	''	956ddba9
THETA AFTER TIMESTEP	☑	0	4	'DALLTH'	'TDMPMN'	'UPMEAN'	''	909bff04
SPECIFIC HUMIDITY AFTER TIMESTEP	☑	0	10	'DALLTH'	'TDMPMN'	'UPMEAN'	''	5c893fff
QCF AFTER TIMESTEP	☑	0	12	'DALLTH'	'TDMPMN'	'UPMEAN'	''	3cb2b218
SNOW AMOUNT OVER LAND AFT TSTP KG/M2	☑	0	23	'DIAG'	'TDMPMN'	'UPMEAN'	''	03faecae
SNOW AMOUNT OVER LAND AFT TSTP KG/M2	☑	0	23	'DIAG'	'TDAYM'	'UPF'	''	873079d4
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN12'	'UPMEAN'	''	0bcb23e5
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN18'	'UPMEAN'	''	0c009a41
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TDMPMN'	'UPMEAN'	''	0c98b824
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN06'	'UPMEAN'	''	1cf005de
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN03'	'UPMEAN'	''	2ee59b2e
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN15'	'UPMEAN'	''	2f5c7179
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN09'	'UPMEAN'	''	4198c86b
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TDAYM'	'UPJ'	''	436d225f
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN00'	'UPMEAN'	''	787fad9c
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TMPMN21'	'UPMEAN'	''	ce82b367
SURFACE TEMPERATURE AFTER TIMESTEP	☑	0	24	'DIAG'	'TDAYM'	'UPA'	''	ff5043e9
BOUNDARY LAYER DEPTH AFTER TIMESTEP	☑	0	25	'DIAG'	'TDMPMN'	'UPMEAN'	''	5054de2f
SURFACE ZONAL CURRENT AFTER TIMESTEP	☑	0	28	'DIAG'	'TDMPMN'	'UPMEAN'	''	5818ccfd
SURFACE MERID CURRENT AFTER TIMESTEP	☑	0	29	'DIAG'	'TDMPMN'	'UPMEAN'	''	b6f52597
LAND MASK (No halo) (LAND=TRUE)	☑	0	30	'DIAG'	'T90DAY'	'UPI'	''	123930b2
LAND MASK (No halo) (LAND=TRUE)	☑	0	30	'DIAG'	'T6HDMPM'	'UPMEAN'	''	b95437e4
FRAC OF SEA ICE IN SEA AFTER TSTEP	☑	0	31	'DIAG'	'TDAYM'	'UPA'	''	136ab65d
FRAC OF SEA ICE IN SEA AFTER TSTEP	☑	0	31	'DIAG'	'TDAYM'	'UPF'	''	ba44c958
FRAC OF SEA ICE IN SEA AFTER TSTEP	☑	0	31	'DIAG'	'TDMPMN'	'UPMEAN'	''	fd29db66
SEA ICE DEPTH (MEAN OVER ICE) M	☑	0	32	'DIAG'	'TDMPMN'	'UPMEAN'	''	68be071a
SEA ICE DEPTH (MEAN OVER ICE) M	☑	0	32	'DIAG'	'TDAYM'	'UPA'	''	a0b3b225
OROGRAPHY (/STRAT LOWER BC)	☑	0	33	'DIAG'	'T6HDMPM'	'UPMEAN'	''	a400a327
OROGRAPHY (/STRAT LOWER BC)	☑	0	33	'DIAG'	'T90DAY'	'UPI'	''	eb4ddaaf
! SULPHUR DIOXIDE EMISSIONS	□	^ 0	^ 58	^ 'DIAG'	^ 'TDMPMN'	^ 'UPMEAN'	^ ''	! 32006d2f
! DIMETHYL SULPHIDE EMISSIONS (ANCIL)	□	^ 0	^ 59	^ 'DIAG'	^ 'TDMPMN'	^ 'UPMEAN'	^ ''	! 4739fe04

Found namelist:run_ukca=l_ukca_ageair

Figure 1: The STASH panel in Rose.



Section	Item	Description	?	#	datat	dumpp	grid	halo	lbvc	levcom	levelf	le
0: Primary fields				80								
1: SW radiation				83								
2: LW radiation				90								
3: BL and surface				139								
4: LS Precipitation				25								
5: Convection				74								
6: Gravity wave drag				16								
8: Hydrology				20								
9: Cloud scheme				0								
10: Dynamics				0								
12: Dynamics advection				0								
13: Diffusion & filtering				0								
14: Energy adjustments				0								
15: Extra dynamics				2								
16: Extra physics				5								
17: Sulphur chem.				0								
19: Vegetation Dist.				0								
20: Public Weather Service Diagnostics				0								
21: Electric				0								
26: River routing				7								
30: Processed clim.				79								
31: LBCs (input)				0								
32: LBCs (driving)				0								
33: Free tracer prog.				0								
34: UKCA				106								
35: Stochastic				0								
36: Free tracer LBCs				0								
37: UKCA LBCs				0								
38: UKCA diag.				5								
39: Nudging				0								

Figure 1: The new STASH requests panel in Rose.

UKCA STASH sections

UKCA actually has 6 STASH sections - these are:

- **Section 34:** This contains the *prognostic* UKCA variables on model theta levels, i.e. all the transported species, and several other fields which are required to be in the restart file.
- **Section 37:** This is for UKCA tracer lateral boundary conditions for use in limited area configurations.
- **Section 38:** This section is for GLOMAP-mode diagnostics on model theta levels.
- **Section 50:** This section is for Chemical diagnostics on model theta levels (or single levels, e.g. surface).
- **Section 51:** This section duplicates all the variables from Section 34, but on pressure levels. To use this section **`l_ukca_chem_plev`** must be set to **true** in the UKCA panel. Additionally, s51i999 must also be output, as this is the Heavyside function that is used to mask missing data from the pressure-level fields (as the UM fieldsfile format has missing data set to zero).
- **Section 52:** This section duplicates all the variables from Section 50, but on pressure levels. To use this section **`l_ukca_asad_plev`** must be set to **true** in the UKCA panel. Additionally, s51i999 must also be output, as this is the Heavyside function that is used to mask missing data from the pressure-level fields (as the UM fieldsfile format has missing data set to zero).

Viewing Output

For more detailed plotting, tools such as the Iris (http://scitools.org.uk/iris/) and cf-python (http://cfpython.bitbucket.org/) libraries can be used to view UM file formats directly. However, for quick viewing, Xconv (http://badc.nerc.ac.uk/help/software/xconv/) is a very useful tool.

- Output files in 64-bit fieldsfile format can be found (on ARCHER) in

  `/work/n02/n02/`**`$USER`**`/cylc-run/`**`[SUITE-ID]`**`/share/data/History_Data`
  Files often have the following naming convention

  `[SHORT SUITE-ID]``a.p`**`[abcdefghijkmsyx]`**`YYYYMMDD`

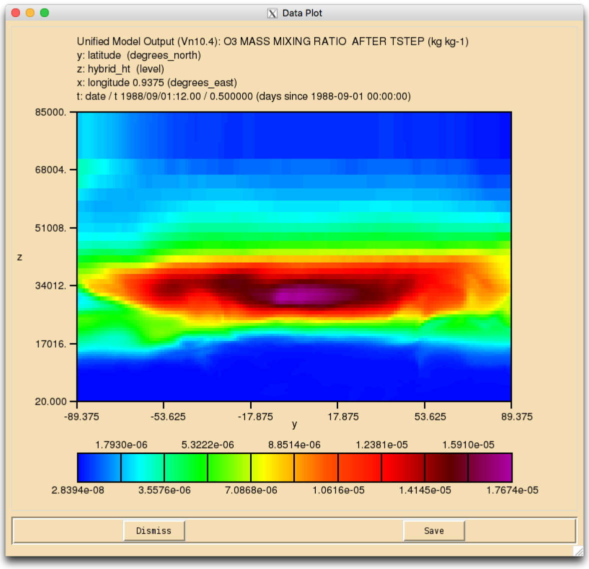
  e.g. `ag308a.pk19880901`

To view these files, do

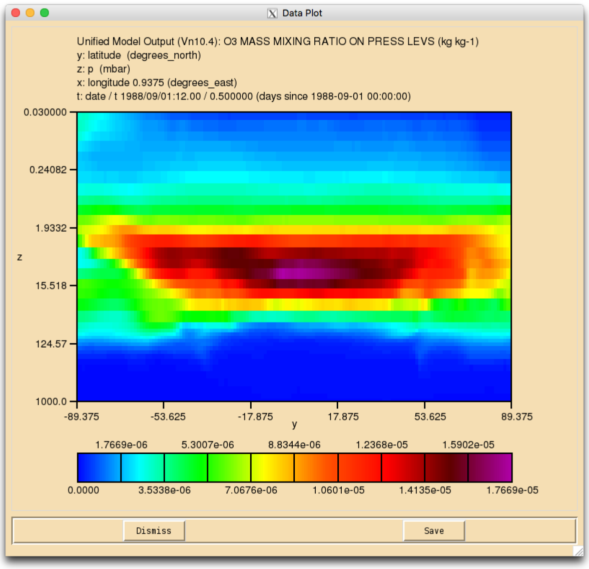
```
xconv ai084a.pk19880901
```

As well as viewing files, you can use Xconv to convert these files to netCDF, by filling in the ***Output file name:*** box (e.g. *foo.nc*), and then clicking **convert**. If no path is defined, this will save the file in the same directory that you opened Xconv from.

Solution to Task 3.1



UKCA Ozone on model levels (y-z)



UKCA Ozone on pressure levels (y-log(z))

You were given the task

- *Output the daily-mean UKCA ozone (section 34 item 001) field to the **UPK** output stream, and then add-in the equivalent diagnostic on pressure levels using the DP36CCM domain*

and were given the hints

- *You will need to remember to run the TidyStashTransform macro once you have added the diagnostics in the STASH panel.*
- *You will need to output the Heavyside function from the pressure-level diagnostics section, otherwise you will get an error.*
- *You will need to set the `l_ukca_chem_plev` logical to **true**.*

For a working Rose suite that has completed this task, please see **`u-ai084@25605`**

The specific Rose changes made are:

```
Index: trunk/app/um/rose-app.conf
===================================================================
--- trunk/app/um/rose-app.conf  (revision 25590)
+++ trunk/app/um/rose-app.conf  (revision 25605)
@@ -3980,7 +3980,7 @@
 l_ukca_arg_act=.true.
 l_ukca_asad_plev=.false.
 l_ukca_chem_aero=.true.
-l_ukca_chem_plev=.false.
+l_ukca_chem_plev=.true.
 !!l_ukca_classic_hetchem=.false.
 !!l_ukca_dust=.false.
 l_ukca_h2o_feedback=.false.
@@ -4438,6 +4438,14 @@
 tim_name='TDAYM'
 use_name='UPA'

+[namelist:streq(0aa62e5d)]
+dom_name='DALLTH'
+isec=34
+item=1
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(0afcd4f8)]
 dom_name='DIAG'
 isec=3
@@ -7726,6 +7734,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(98e19859)]
+dom_name='DP36CCM'
+isec=51
+item=999
```

```
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(990c821b)]
 dom_name='DIAG'
 isec=5
@@ -8070,6 +8086,14 @@
 tim_name='TMPMN18'
 use_name='UPMEAN'

+[namelist:streq(aa677761)]
+dom_name='DP36CCM'
+isec=51
+item=1
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(ac464bf5)]
 dom_name='DIAG'
 isec=2
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task3.1/task3.1.rose.diff** on PUMA.

If you open the **.pk** file in Xconv, you should see the following fields:

```
0    : 192   144   36    1     O3 MASS MIXING RATIO
1    : 192   144   36    1     Molar flux density
2    : 192   144   85    1     O3 MASS MIXING RATIO
```

Sample output from this task can be found at **/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task3.1/ai084a.pk19880901** on ARCHER.

Tutorial 4

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UKCA Chemistry and Aerosol vn10.4 Tutorial 4

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will do in this tutorial

In this tutorial you will learn how to make the required changes in Rose and in UKCA to include new chemical tracers. As you learn how to do this you will add two new tracers to the UKCA tutorial suite you have already been running.

Task 4.1: Add new tracers into Rose and UKCA

TASK4.1: Add in two new tracers in to slots 64 and 65 for the StratTrop chemistry scheme. The tracer in slot 64 will be called **ALICE** and the tracer in slot 65 will be called **BOB** and initialise these tracers to `1.000000e-12`. You should also output these two tracers through the **UPK** stream in STASH as daily means. In UKCA, you should set the conversion factor for each of these to 1.0.

Make a branch

As UKCA is a framework, it must have the infrastructure around it to allow it to work, with the infrastructure being the UM itself. In this tutorial you will add in two new chemical tracers. In this past this was done in two steps, but in Rose this must be done in a single step from vn10.6 onwards. Even though these tutorials are at vn10.4, we will follow the same steps as for vn10.6.

For this tutorial you will need to make a new branch in the usual way. You should do this now.

You will have learned how to make UM branches in the NCAS-CMS FCM Tutorial (https://puma.nerc.ac.uk/trac/UM_TUTORIAL) . However, now you should use um.x_tr as the source of your branch.

For example, first you should make a ticket on the Met Office SRS Trac pages (https://code.metoffice.gov.uk/trac/um/newticket) (login required) and then make the branch like so

```
fcm branch-create --type dev -k ticket_number your_branch_name fcm:um.x_tr@vn10.4
```

before checking-out your branch by

```
fcm checkout fcm:um.x_br/dev/userid/vn10.4_your_branch_name
```

More information on FCM can be found at the NCAS-CMS FCM pages (http://cms.ncas.ac.uk/wiki/Fcm) or the FCM User Guide (http://metomi.github.io/fcm/doc/user_guide/)

Metadata

In Rose, the GUI appearance is controlled by *metadata*, and it is possible to edit this metadata to add new variables to panels. We will not do this in this tutorial, but you will need to change where Rose looks for metadata, as the STASHmaster_A is also metadata.

vn10.4

At vn10.4, the um metadata associated with your suite can be found by clicking on the **um** menu entry. In the base suite, this is set to **`/home/grenville/meta/ga7_vn10.4`**. However, you will also need to include the metadata changes here. To do this, cd into your branch and merge-in the branch **`fcm:um.x_br/dev/lukeabraham/vn10.4_ga7_meta`**

```
fcm merge fcm:um.x_br/dev/lukeabraham/vn10.4_ga7_meta
```

and then

```
fcm commit
```

vn10.6+

At vn10.6, this is not necessary, as the additional metadata for GA7.0 is already in the trunk.

Using your new metadata within Rose

To pick-up the metadata changes, you should edit the **meta** path in **um** to point to

```
um-atmos/HEAD
```

From now on, when you want to open your Rose suite for editing, instead of doing it through rosie, you should instead open the job for editing by going to your `$HOME/roses/`**`[SUITE-ID]`** directory, and opening it using the command

```
rose edit -M /path/to/vn10.4_your_branch_name/rose-meta
```

If you don't do this, the STASHmaster changes will not be picked up, and you won't be able to select the tracers.

Rose Changes

Include your branch for code changes

Although we haven't made any code changes yet, you will (at some point) need to include your branch in Rose so that the UKCA code changes can be picked-up and compiled. To do this go to **fcm_make_um** ⟶ **env** ⟶ **Sources** and add a new branch by clicking the **plus symbol** in the **um_sources** section. You should then put

```
/path/to/vn10.4_your_branch_name
```

if you wish to run from a working copy, and

```
branches/dev/[your MOSRS username]/vn10.4_your_branch_name
```

if you want to run from the repository. You can specify specific revision numbers by putting `@`**`REV`** at the end of this line (where **REV** is the revision number, e.g. 12345 etc.).

STASHmaster_A

In Rose-based jobs, adding new UKCA tracers is done through editing the STASHmaster_A file directly. Take a look at the **STASHmaster_A** file, found in

```
/path/to/vn10.4_your_branch_name/rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A
```

This is a large file, as it contains all the possible STASH items. Scroll down the file until you get to section 34, and you will see how the tracers are defined. The key entries to consider are highlighted in **red**. All entried are **fixed-width**, so when editing the file, ensure not to change the spacing, otherwise you will get errors.

```
#===============================================================================
# Section 34 UKCA Chemistry
#===============================================================================
#
1|    1 |   34 |    1 |O3 MASS MIXING RATIO AFTER TIMESTEP |
2|    2 |    0 |    1 |    1 |    2 |   40 |   11 |    0 |    0 |    0 |    0 |
3| 000000000000000000000000111110 | 00000000000000000001 |    1 |
4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
5|    0 | 2101 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
#
```

The meaning of these entries is:

First Line:

- **34:** The *STASH section*, in this case Section 34, UKCA prognostics.
- **1:** The *STASH item*, in this case, the first item in s34, ozone.

- **O3 MASS MIXING RATIO AFTER TIMESTEP:** The *name* of the field in the STASHmaster file. This can be anything descriptive, but it isn't read by the model, and is only considered in Rose (or e.g. Xconv).
-

Second Line:

- **2:** The *Space Code*, which tells the UM whether the field should be held in the restart dump or not. For prognostics, this should be 2 (which means that they should be stored in the restart dump), but for diagnostics that are only passed to output files, this should be 0.

Third Line:

- **000000000000000000000000111110:** These are *Options Codes* which determine which scheme the STASH field (i.e. tracer in this case) are valid for. These are counted from the **right**, ***n1*** to ***n30***, and for UKCA only the first 8 are used. These have the following meaning:
  - **n1:** Age-of-air tracer (*ageair*) or aerosol tracers
  - **n2:** Standard Tropospheric Chemistry scheme using the Backward Euler solver (*trop*)
  - **n3:** Regional Air Quality Chemistry scheme using the Backward Euler solver (*raq*)
  - **n4:** Tropospheric Chemistry with Isoprene scheme using the Newton-Raphson solver (*tropisop*)
  - **n5:** Stratospheric-Tropospheric Chemistry using the Newton-Raphson solver (*strattrop*, also know as *CheST*)
  - **n6:** Standard Stratospheric Chemistry using the Newton-Raphson solver (*strat*)
  - **n7:** Offline-oxidants scheme (to drive GLOMAP-mode) using the Newton-Raphson solver (*offline*)
  - **n8:** Offline-oxidants scheme (to drive GLOMAP-mode) using the Newton-Raphson solver (*offline_be*)

Therefore, looking at the option code for ozone (s34i001), it is valid for the trop, raq, tropisop, strattrop, and strat chemistry schemes.

Fifth Line:

- **2101:** This is the *PP Field Code* and should be unique to each tracer. Here these begin counting at 2101 (s34i001) and end at 2250 (s34i150) for vn10.4, or 2356 (s34i256) for vn10.6, as the number of tracers has been increased.

So to make a STASH entry for a single tracer called ALICE in slot s34i064 that is only valid in the StratTrop scheme, the STASHmaster_A entry would look like

```
#
1|    1 |   34 |   64 |ALICE MASS MIXING RATIO AFTER TSTEP |
2|    2 |    0 |    1 |    1 |    2 |   40 |   11 |    0 |    0 |    0 |    0 |
3| 000000000000000000000000010000 | 00000000000000000001 |    1 |
4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
5|    0 | 2164 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
#
```

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

You should make these changes to STASHmaster_A, and then **`fcm commit`** these changes. This is important, otherwise ARCHER will not be able to see the changes you have made once you have included your new STASHmaster_A file in Rose.

Section 51

All STASH entries in Section 34 need a corresponding pressure-level field to be added to section 51. The equivalent STASHmaster_A entry for s51 ozone is:

```
#
#===============================================================================
# Section 51 UKCA Chemistry on pressure levels
#===============================================================================
#
1|    1 |   51 |    1 |O3 MASS MIXING RATIO ON PRESS LEVS   |
2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
3| 000000000000000000000000111110 | 00000000000000000001 |    3 |
4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
5|    0 | 2101 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
#
```

You will notice that there are a number of changes to various codes, and this is to do with defining the grid that the diagnostic is valid on, whether it can be held in the dump, etc. For more information on what these codes mean, please see Appendix C in UMDP C4, which can be obtained from the SRS here (password required) (https://code.metoffice.gov.uk/doc/um/latest/umdp.html) . When making a new entry, the easiest thing to do is copy an existing entry and make the required changes to the item, name, PP field code, and option codes.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

Help text

You should also add appropriate help text into the **`vn10.4_your_branch_name/rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf`** file, e.g.

```
[stashmaster:code(34064)]
description=ALICE MASS MIXING RATIO AFTER TIMESTEP
help=UKCA Tutiorial Tracer ALICE Mass Mixing Ratio in kg/kg(Air)
```

and

```
[stashmaster:code(51064)]
description=ALICE  MASS MIX RATIO ON PRESS LEVS
help=UKCA Tutiorial Tracer ALICE Mass Mixing Ratio in kg/kg(Air)
    =on pressure levels
```

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

Use your new STASHmaster file in Rose

To get Rose to recognise your STASHmaster file, you will need to make a number of changes:

1. Point the **um** metadata to **um-atmos/HEAD** and edit Rose using `rose edit -M /path/to/vn10.4_your_branch_name/rose-meta` (you should already be doing this after following the instructions in the metadata section above.
2. You need to open the `$HOME/roses/[SUITE-ID]/app/um/rose-app.conf` file in a text editor (e.g. vim, emacs, nedit etc.) and add the line `STASHMSTR=STASHmaster` inside the `[env]` block
3. You need to open the `$HOME/roses/[SUITE-ID]/rose-suite.conf` file in a text editor and add the following lines at the top of the file:

```
[file:app/um/file/STASHmaster]
source=fcm:um.xm_br/dev/[your MOSRS userid]/vn10.4_your_branch_name/rose-meta/um-atmos/HEAD/etc/stash/STASHmaste
```

> You need to ensure that you have committed your STASHmaster_A changes, otherwise your new tracer(s) will not be seen on ARCHER during the reconfiguration or atmosphere steps.

Initialise your new tracer(s)

Your new tracer(s) is a prognostic variable, as therefore the UM requires prior knowledge of the values it has to be able to run properly. To do this you need to go to **um** ⟶ **namelist** ⟶ **Reconfiguration and Ancillary Control** ⟶ **Configure ancils and initialise dump fields**. Here you will see a list of fields. You can change the order of these by e.g. STASH number, as this often makes it easier to view.

To add new fields, right click anywhere within the table and click **Add new section**. This will make a new entry with index **1**, if you add another entry, it will be given index **2** etc.. Right-click on this and click on **View namelist:items(*X*)** (where ***X*** is the index number). This will open a new tab where you can select the STASH section and item for the field you want to initialise using the drop-down menus. Some UKCA tracers need to be given full 3D initial conditions in ancillary file format. However, for this example we will initialise the tracer to a small number, 1.000000×10^{-12}. To do this, select the radio button for **Set to a specified constant value** and put **1.000000e-12** in the dialog box labelled **user_prog_rconst** at the bottom of the panel.

You will need to do this for each of the tracers you are adding. When you have finished, you will need to go to the **STASH Requests** panel (see the STASH tutorial) and run the **TidyStashTransform** macro to correctly generate the required index value for each tracer initialisation.

At this point, a vn10.4 job (in fact, all Rose jobs prior to vn10.5) will be able to run and output these tracers. However, at vn10.6 the number of tracers was increased to 256, and when doing this extra checks were included that prevented jobs from running with s34 tracers turned on, but without UKCA using them. Because of this we will also include the UKCA changes now as well.

Output your new tracers

To output your tracers, go to the **STASH panel** and output your tracers as described in the What is STASH? tutorial.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

Required UKCA Code Changes

`ukca_set_nmspec.F90`

Inside UKCA there is a master mapping array that tells the UKCA code which transported species are placed into a particular item number in section 34. At vn10.4 these are contained in the first 150 slots, and at vn10.6 these are in the first 256 slots.

This array is called **`nm_spec`**, and it can be found in `ukca_set_nmspec.F90`. At vn10.4, it looks like this:

```
nm_spec(1:a_max_ukcavars) = (/                                     &
'O3        ','NO        ','NO3       ','NO2       ','N2O5      ',  &
'HO2NO2    ','HONO2     ','H2O2      ','CH4       ','CO        ',  & !10
'HCHO      ','MeOOH     ','HONO      ','C2H6      ','EtOOH     ',  &
'MeCHO     ','PAN       ','C3H8      ','n-PrOOH   ','i-PrOOH   ',  & !20
'EtCHO     ','Me2CO     ','MeCOCH2OOH','PPAN      ','MeONO2    ',  &
'O3_S      ','C5H8      ','ISOOH     ','ISON      ','MACR      ',  & !30
'MACROOH   ','MPAN      ','HACET     ','MGLY      ','NALD      ',  &
'HCOOH     ','MeCO3H    ','MeCO2H    ','H2O       ','ISO2      ',  & !40
'Cl        ','ClO       ','Cl2O2     ','OClO      ','Br        ',  &
'BrO       ','BrCl      ','BrONO2    ','N2O       ','HCl       ',  & !50
'HOCl      ','HBr       ','HOBr      ','ClONO2    ','CFCl3     ',  &
'CF2Cl2    ','MeBr      ','N         ','O(3P)     ','MACRO2    ',  & !60
'MeCl      ','CF2ClBr   ','CCl4      ','CF2ClCFCl2','CHF2Cl    ',  &
'MeCCl3    ','CF3Br     ','H2OS      ','CH2Br2    ','H2        ',  & !70
'DMS       ','SO2       ','H2SO4     ','MSA       ','DMSO      ',  &
'NH3       ','CS2       ','COS       ','H2S       ','H         ',  & !80
'OH        ','HO2       ','MeOO      ','EtOO      ','MeCO3     ',  &
'n-PrOO    ','i-PrOO    ','EtCO3     ','MeCOCH2OO ','MeOH      ',  & !90
'Monoterp  ','Sec_Org   ','SESQUITERP','SO3       ','AROM      ',  &
'O(3P)_S   ','O(1D)_S   ','NO2       ','BrO       ','HCl       ',  & !100
'Nuc_SOL_ND','Nuc_SOL_SU','Ait_SOL_ND','Ait_SOL_SU','Ait_SOL_BC',  &
'Ait_SOL_OC','Acc_SOL_ND','Acc_SOL_SU','Acc_SOL_BC','Acc_SOL_OC',  & !110
'Acc_SOL_SS','Acc_SOL_DU','Cor_SOL_ND','Cor_SOL_SU','Cor_SOL_BC',  &
'Cor_SOL_OC','Cor_SOL_SS','Cor_SOL_DU','Ait_INS_ND','Ait_INS_BC',  & !120
'Ait_INS_OC','Acc_INS_ND','Acc_INS_DU','Cor_INS_ND','Cor_INS_DU',  &
'Nuc_SOL_OC','Ait_SOL_SS','Nuc_SOL_SO','Ait_SOL_SO','Acc_SOL_SO',  & !130
'Cor_SOL_SO','Nuc_SOL_NH','Ait_SOL_NH','Acc_SOL_NH','Cor_SOL_NH',  &
'Nuc_SOL_NT','Ait_SOL_NT','Acc_SOL_NT','Cor_SOL_NT','XXX       ',  & !140
'Anth_Prec ','Bio_Prec  ','Anth_Cond ','Bio_Cond  ','XXX       ',  &
'XXX       ','XXX       ','XXX       ','PASSIVE O3','AGE OF AIR'   & !150
 /)
```

This array is **case sensitive** and each string is a **fixed length** of **10 characters**, with the whitespace being made up of spaces and not another tpye of white space (e.g. tabs).

When adding new tracers you should not overwrite tracers that are already in use by the chemistry scheme that you are using (e.g. StratTrop etc.), and it is best to also take care and avoid tracers in use by other schemes, if possible. You can see the tracers used by each scheme by looking in the `chch_defs` array at the top of each `ukca_chem_scheme.F90` (e.g. `ukca_chem_strattrop.F90` etc.).

Here you should put a new species, `'ALICE     '`, into tracer slot 64 (current specified as `'CF2ClCFCl2'`, which is not in use by any scheme at the moment).

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

ukca_chem_*scheme*.F90

We will go through changes that need to be made for the StratTrop chemistry scheme (defined in the file **`ukca_chem_strattrop.F90`**), but equivalent changes would need to be made for others, e.g. TropIsop or Strat. For this example we will only refer to this scheme.

In this file the list of species used in chemistry is defined by the array **`chch_defs_strattrop`**. In fact, there are two copies of this list, **`chch_defs_strattrop_chem`** and **`chch_defs_strattrop_aer`**. This is due to some slight differences when adding in the required chemistry to drive GLOMAP-mode. The list of species is held in a *derived type*, of the format:

```
chch_t( N,'SPECIES   ',  X,'TYPE      ','FAMILY    ',  D,  W,  E),  &
```

Where:

- **`N`** is a dummy integer. The value doesn't really matter, although it is usually used to number the species in the list.
- **`'SPECIES   '`** is the name of the species, e.g. `'O3        '`
- **`X`** number of odd atoms
- **`'TYPE      '`** describes whether the species is a tracer (`'TR        '`), a steady-state species (`'SS        '`), a constant (`'CT        '`), or a constant field (`'CF        '`). For SS, CT, and CF, special code will need to be added.
- **`'FAMILY    '`** is the family that the species belongs to. This field is not currently used.
- **`D`** is **1** if the species is dry-deposited, and **0** otherwise.
- **`W`** is **1** if the species is wet-deposited, and **0** otherwise.
- **`E`** is **1** if the species is emitted, and **0** otherwise. This field is not currently used.

Therefore to add-in the ALICE species, we should insert a line similar to this one

```
chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  1)   &
```

into **`chch_defs_strattrop_chem`** and **`chch_defs_strattrop_aer`**, remembering to also **increment the size of these arrays**

When inserting the tracer into **`chch_defs_strattrop_aer`**, some care must be taken if you also want the species to be dry and/or wet deposited at some point, as the arrays that define these are order specific. It is best therefore to insert the tracer into the equivalent place in both `chch_defs_strattrop`, which will often mean inserting them before the aerosol-chemistry-specific species (i.e. DMS, SO2, H2SO4, MSA, DMSO, NH3, CS2, COS, H2S, SO3, Monoterp, and Sec_Org). If the tracers that you are adding are only going to be a part of the aerosol chemistry used to drive GLOMAP-mode, then it is fine to just edit the `chch_defs_strattrop_aer` array and put them at the end of the list.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

ukca_setd1defs.F90

In **`ukca_setd1defs.F90`** you will find code blocks which set values for various parameters depending on the scheme used. In this example you will need to scroll down to the section which defines the **StratTrop** (also known as *CheST*) chemistry, which is located in the *Stratospheric Chemistry* section and is referenced by using the **`L_ukca_strattrop`** logical.

The IF block tests against `L_ukca_strattrop` and `L_ukca_achem` (which determines whether or not you require the additional chemistry used to drive the GLOMAP-mode aerosol scheme). You should increment the value of **`n_chem_tracers`** by the number of chemical tracers that you are adding in the correct sections of the IF block.

For example, if you only added the tracers to `chch_defs_strattrop_aer` (and are only interested in using these new tracers with GLOMAP-mode turned on) then you only need to edit the value of `n_chem_tracers` in the `(L_ukca_strattrop .AND. L_ukca_achem)` section etc.

If you are adding to a different chemistry scheme then you will need to make these changes accordingly.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

ukca_constants.F90

The unit of the tracers is kg(species)/kg(air) (i.e. mass mixing ratio, or **mmr**), but inside UKCA these species are converted to volume mixing ratio (or **vmr**). To enable UKCA to do this you will need to add the conversion factor(s) for your new tracer(s) into the code. This is done in the **`ukca_constants.F90`** module.

Open this file and add the required conversion factor(s). The naming convention for these is **M_species** is the molecular mass of the new species in g/mol, and **C_species** for the converson factor from vmr to mmr (calculated as M_species/M_air, where M_air=28.97). In actuality, only the C_species listing is always required, although you may need to add the M_species value later if you are emitting into the new species that you are adding.

For example:

```
REAL, PARAMETER :: C_ALICE      = 1.0000
```

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

`ukca_cspecies.F90`

After you have added in the **C_species** conversion factors, you will need to tell UKCA to use them for your species. To do this you need to edit the **ukca_cspecies.F90** module, which contains code which contructs the **c_species** array of conversion factors for the advected tracers. This contains a subroutine called `ukca_calc_cspecies` which has a long block of code that you need to edit to add an entry like this:

```
WHERE (advt == 'ALICE     ') c_species = C_ALICE
```

The **advt** array is automatically generated by UKCA at run-time from the `chch_defs_scheme` chemistry scheme definition you edited earlier, so your new tracer(s) will exist within it. You need to add in a new line for each of your tracers which sets the value of the **c_species** array to your individual C_species parameter. Add the line(s) in at the end of the block.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

`ukca_setup_chem_mod.F90`

The changes made to `ukca_setd1defs.F90` told UKCA how many tracers to expect in Section 34. However, you also need to tell UKCA how many new species you have, and how many of them are tracers. While you have added code to `ukca_chem_scheme.F90` (e.g. `ukca_chem_strattrop.F90`), you also need to tell the chemical solver how many species and tracers to expect.

This is done in the routine **`ukca_setup_chem_mod.F90`**. Within this routine is a large CASE statement that is used to define various parameters used by the chemical solver. For the StratTrop scheme you should find the section referenced by

```
CASE (i_ukca_chem_strattrop)
```

and you should increment the values of **`jpctr`** (which defines the number of tracers used in the scheme) and **`jpspec`** (which defines the number of species used in the scheme, and also includes steady-state and constant species) by the number of tracers you have added.

Remember: You need to add **2** tracers, ALICE in s34i064 and BOB in s34i065.

Run your suite

Now that you have made the required changes to Rose and in your branch, please run your suite. You may find that it fails on the, `fcm_make2_um`, `recon`, or `atmos_main` jobs. To find the errors and see output, you should go to the

```
$HOME/[your ARCHER userid]/cylc-run/[SUITE-ID]
```

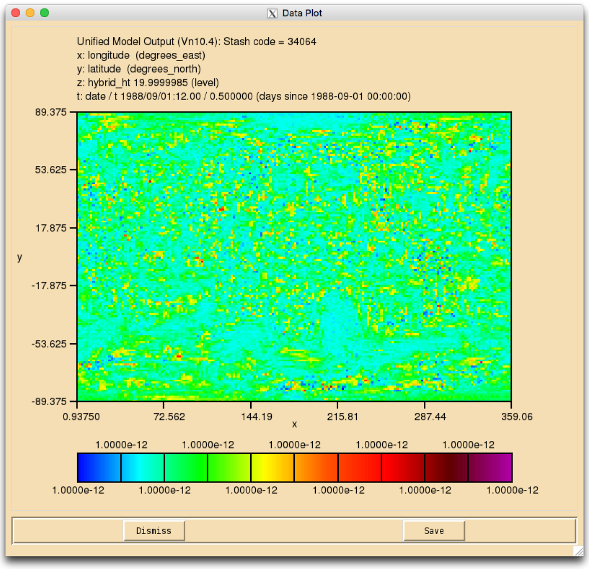
directory on ARCHER. Within this there are a number of directories. To see the log files, cd into

```
log/job/X/[JOB NAME]/NN
```

(where X will be either *19880901T0000Z* on ARCHER, or may be *1* if you are using a vn10.6 suite based on a Rose stem testing job) and view the job.err or job.out files. When the suite successfully runs, the fieldsfile output can usually be found in

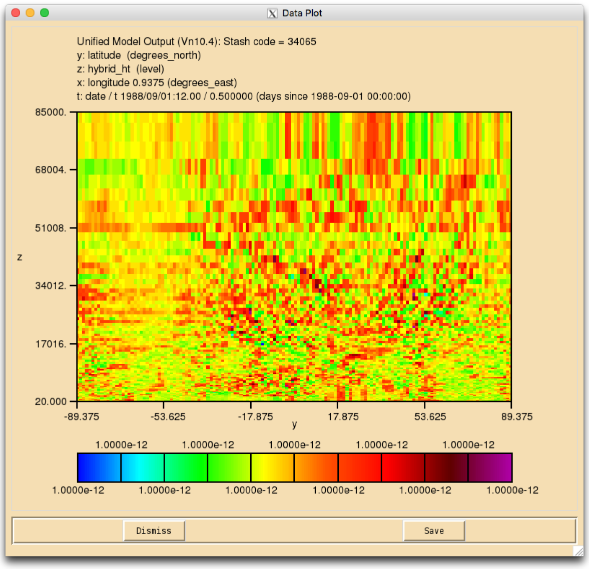
```
$HOME/[your ARCHER userid]/cylc-run/[SUITE-ID]/share/data/History_Data
```

Numerical Noise



```
Unified Model Output (Vn10.4): Stash code = 34064
x: longitude  (degrees_east)
y: latitude  (degrees_north)
z: hybrid_ht 19.9999985 (level)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)
```

Numerical noise in the ALICE tracer (s34i064)



```
Unified Model Output (Vn10.4): Stash code = 34065
y: latitude  (degrees_north)
z: hybrid_ht  (level)
x: longitude 0.9375 (degrees_east)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)
```

Numerical noise in the BOB tracer (s34i065)

When your suite has run successfully, and you view the fields for your new tracer(s) in Xconv, you may find that they have a speckled appearance, rather than being constant. This is due to numerical noise that has been introduced as the tracer is run through the UKCA chemical solver. Once the field is converted to 32-bit this should disappear. It will also cease to become apparent when emissions and reactions are applied to these tracers.

Solution to Task 4.1

You were given the task

- *Add in two new tracers in to slots 64 and 65 for the StratTrop chemistry scheme. The tracer in slot 64 will be called **ALICE** and the tracer in slot 65 will be called **BOB** and initialise these tracers to `1.000000e-12`. You should also output these two tracers through the **UPK** stream in STASH as daily means. In UKCA, you should set the conversion factor for each of these to 1.0.*

For a working Rose suite that has completed this task, please see **`u-ai084@25815`**

The specific Rose changes made are:

```
Index: trunk/app/um/rose-app.conf
===================================================================
--- trunk/app/um/rose-app.conf  (revision 25605)
+++ trunk/app/um/rose-app.conf  (revision 25815)
@@ -1,4 +1,4 @@
-meta=/home/grenville/meta/ga7_vn10.4
+meta=um-atmos/HEAD

 [command]
 default=um-atmos
@@ -23,6 +23,7 @@
 RECON_KEEP_MPP_STDOUT=true
 RECON_STDOUT_FILE=pe_output/${RUNID}.fort6.pe
 SPECTRAL_FILE_DIR=$UMDIR/vn$VN/ctldata/spectral/ga7
+STASHMSTR=STASHmaster
 UM_THREAD_LEVEL=MULTIPLE
 VN=10.4

@@ -1973,6 +1974,17 @@
 !!user_prog_ancil_stash_req=
 user_prog_rconst=1.000000e-18

+[namelist:items(8dd1e33d)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
+source=6
+stash_req=34064
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+user_prog_rconst=1.000000e-12
+
 [namelist:items(8f0cb76a)]
 ancilfilename='$CHEM_INIT_FILE'
 domain=1
@@ -2281,6 +2293,17 @@
 !!user_prog_ancil_stash_req=
 user_prog_rconst=1.000000e-18

+[namelist:items(d9a844ee)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
+source=6
+stash_req=34065
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+user_prog_rconst=1.000000e-12
+
 [namelist:items(dc674670)]
 ancilfilename='$CHEM_INIT_FILE'
 domain=1
@@ -4574,6 +4597,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(114ee958)]
+dom_name='DALLTH'
+isec=34
+item=64
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(1177a86c)]
 dom_name='DIAG'
 isec=2
@@ -5838,6 +5869,14 @@
 tim_name='TALLTS'
 use_name='UPUKCA'

+[namelist:streq(4455fd38)]
+dom_name='DALLTH'
+isec=34
+item=65
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(44a86587)]
 dom_name='DPFTS'
 isec=3
Index: trunk/app/fcm_make_um/rose-app.conf
===================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 25605)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 25815)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
Index: trunk/rose-suite.conf
===================================================================
--- trunk/rose-suite.conf       (revision 25605)
+++ trunk/rose-suite.conf       (revision 25815)
@@ -1,3 +1,6 @@
+[file:app/um/file/STASHmaster]
+source=fcm:um.xm_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns/rose-meta/um-atmos/HEAD/etc/stash/STASHmaster@HE
+
 [jinja2:suite.rc]
 !!ACCOUNT_USR='foundation'
 ANCIL_OPT_KEYS=
```

For a working UM branch that has completed this task, please see **fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@30979**

The specific UM changes made are:

```

Index: src/atmosphere/UKCA/ukca_setd1defs.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setd1defs.F90      (revision 30974)
+++ src/atmosphere/UKCA/ukca_setd1defs.F90      (revision 30979)
```

```
@@ -309,7 +309,7 @@
         (/'NO        ','CH4       ','CO        ','HCHO      ', &
           'C2H6      ','C3H8      ','Me2CO     ','MeCHO     ', &
           'C5H8      ','NO_aircrft'/)
-    n_chem_tracers = 71         ! No chem tracers
+    n_chem_tracers = 73         ! No chem tracers
     nr_therm       = 220        ! thermal reactions
     nr_phot        = 55         ! photolytic (ATA)

@@ -325,7 +325,7 @@
           'SO2_high  ','NH3       ','DMS       ','SO2_nat   ', &
           'BC_biomass','OC_biomass','NO_aircrft'/)
     n_aero_tracers = 12
-    n_chem_tracers = 71         ! No chem tracers
+    n_chem_tracers = 73         ! No chem tracers
     IF (L_ukca_trophet) THEN
       nr_therm     = 241        ! thermal reactions
     ELSE
Index: src/atmosphere/UKCA/ukca_set_nmspec.F90
===================================================================
--- src/atmosphere/UKCA/ukca_set_nmspec.F90     (revision 30974)
+++ src/atmosphere/UKCA/ukca_set_nmspec.F90     (revision 30979)
@@ -73,7 +73,7 @@
 'BrO       ','BrCl      ','BrONO2    ','N2O       ','HCl       ',  & !50
 'HOCl      ','HBr       ','HOBr      ','ClONO2    ','CFCl3     ',  &
 'CF2Cl2    ','MeBr      ','N         ','O(3P)     ','MACRO2    ',  & !60
-'MeCl      ','CF2ClBr   ','CCl4      ','CF2ClCFCl2','CHF2Cl    ',  &
+'MeCl      ','CF2ClBr   ','CCl4      ','ALICE     ','BOB       ',  &
 'MeCCl3    ','CF3Br     ','H2OS      ','CH2Br2    ','H2        ',  & !70
 'DMS       ','SO2       ','H2SO4     ','MSA       ','DMSO      ',  &
 'NH3       ','CS2       ','COS       ','H2S       ','H         ',  & !80
Index: src/atmosphere/UKCA/ukca_constants.F90
===================================================================
--- src/atmosphere/UKCA/ukca_constants.F90      (revision 30974)
+++ src/atmosphere/UKCA/ukca_constants.F90      (revision 30979)
@@ -272,6 +272,10 @@
 REAL, PARAMETER :: c_isosvoc2   = 2.3473   ! as C5H8
 REAL, PARAMETER :: c_isosoa     = 4.4874   ! 130.0

+!     UKCA Tutorial tracers
+REAL, PARAMETER :: C_ALICE      = 1.0000
+REAL, PARAMETER :: C_BOB        = 1.0000
+
 !     molecular masses in g/mol of emitted species,
 !     for budget calculations
 REAL, PARAMETER :: m_ho2     =  33.007
Index: src/atmosphere/UKCA/ukca_chem_strattrop.F90
===================================================================
--- src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 30974)
+++ src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 30979)
@@ -63,7 +63,7 @@


 ! ATA NLA CheST Chemistry v1.2
-TYPE(chch_t), PUBLIC :: chch_defs_strattrop_chem(1:75)=(/            &
+TYPE(chch_t), PUBLIC :: chch_defs_strattrop_chem(1:77)=(/            &
 !   1
 chch_t(  1,'O(3P)     ',  1,'TR        ','Ox        ',  0,  0,  0),  &
 !   2
@@ -213,10 +213,14 @@
 !  74
 chch_t( 74,'O2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  75
-chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0)   &
+chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
+!  76
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  0),  &
+!  77
+chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0)   &
   /)

-TYPE(chch_t), PUBLIC :: chch_defs_strattrop_aer(1:87)=(/             &
+TYPE(chch_t), PUBLIC :: chch_defs_strattrop_aer(1:89)=(/             &
 !   1
 chch_t(  1,'O(3P)     ',  1,'TR        ','Ox        ',  0,  0,  0),  &
 !   2
@@ -367,30 +371,34 @@
 chch_t( 74,'O2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  75
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
-!  76
-chch_t( 76,'DMS       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  77 DD:37,WD:31,EM:10
-chch_t( 77,'SO2       ',  1,'TR        ','          ',  1,  1,  1),  &
+!  76
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  0),  &
+!  77
+chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0),  &
 !  78
-chch_t( 78,'H2SO4     ',  1,'TR        ','          ',  0,  0,  0),  &
-!  79
-chch_t( 79,'MSA       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  80 DD:38,WD:32
-chch_t( 80,'DMSO      ',  1,'TR        ','          ',  1,  1,  0),  &
-!  81 DD:39,WD:33,EM:11
-chch_t( 81,'NH3       ',  1,'TR        ','          ',  1,  1,  1),  &
-!  82
-chch_t( 82,'CS2       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  83
-chch_t( 83,'COS       ',  1,'TR        ','          ',  0,  0,  0),  &
+chch_t( 78,'DMS       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  79 DD:37,WD:31,EM:10
+chch_t( 79,'SO2       ',  1,'TR        ','          ',  1,  1,  1),  &
+!  80
+chch_t( 80,'H2SO4     ',  1,'TR        ','          ',  0,  0,  0),  &
+!  81
+chch_t( 81,'MSA       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  82 DD:38,WD:32
+chch_t( 82,'DMSO      ',  1,'TR        ','          ',  1,  1,  0),  &
+!  83 DD:39,WD:33,EM:11
+chch_t( 83,'NH3       ',  1,'TR        ','          ',  1,  1,  1),  &
 !  84
-chch_t( 84,'H2S       ',  1,'TR        ','          ',  0,  0,  0),  &
+chch_t( 84,'CS2       ',  1,'TR        ','          ',  0,  0,  0),  &
 !  85
-chch_t( 85,'SO3       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  86 DD:40,      EM: 12
-chch_t( 86,'Monoterp  ',  1,'TR        ','          ',  1,  0,  1),  &
-!  87 DD:41,WD:34
-chch_t( 87,'Sec_Org   ',  1,'TR        ','          ',  1,  1,  0)   &
+chch_t( 85,'COS       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  86
+chch_t( 86,'H2S       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  87
+chch_t( 87,'SO3       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  88 DD:40,      EM: 12
+chch_t( 88,'Monoterp  ',  1,'TR        ','          ',  1,  0,  1),  &
+!  89 DD:41,WD:34
+chch_t( 89,'Sec_Org   ',  1,'TR        ','          ',  1,  1,  0)   &
   /)

 TYPE(ratb_t) :: ratb_defs_strattrop_chem(198)
Index: src/atmosphere/UKCA/ukca_setup_chem_mod.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 30974)
+++ src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 30979)
@@ -248,8 +248,8 @@
   l_ukca_strattrop = .TRUE.
   l_ukca_advh2o    = .TRUE.
   ukca_int_method = int_method_nr
-  jpctr           = 71
-  jpspec          = 75
+  jpctr           = 73
+  jpspec          = 77
   jpbk            = 198
   jptk            = 24
   jppj            = 56
Index: src/atmosphere/UKCA/ukca_cspecies.F90
===================================================================
--- src/atmosphere/UKCA/ukca_cspecies.F90       (revision 30974)
+++ src/atmosphere/UKCA/ukca_cspecies.F90       (revision 30979)
@@ -278,6 +278,9 @@
 WHERE (advt == 'ORGNIT     ') c_species = c_orgnit
 WHERE (advt == 'PASSIVE O3') c_species = 1.0
 WHERE (advt == 'AGE OF AIR') c_species = 1.0
+!     UKCA Tutorial Tracers
+WHERE (advt == 'ALICE     ') c_species = C_ALICE
+WHERE (advt == 'BOB       ') c_species = C_BOB

 ! non-advected tracers
 c_na_species=0.0
Index: rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf
===================================================================
--- rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf (revision 30974)
+++ rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf (revision 30979)
@@ -13144,6 +13144,14 @@
 description=O3P MASS MIXING RATIO AFTER TIMESTEP
 help=Oxygen atom (ground state) Mass Mixing Ratio in kg/kg(Air)
 
+[stashmaster:code(34064)]
+description=ALICE MASS MIXING RATIO AFTER TIMESTEP
+help=UKCA Tutiorial Tracer ALICE Mass Mixing Ratio in kg/kg(Air)
+
+[stashmaster:code(34065)]
+description=BOB MASS MIXING RATIO AFTER TIMESTEP
+help=UKCA Tutiorial Tracer BOB Mass Mixing Ratio in kg/kg(Air)
+
 [stashmaster:code(34070)]
 description=H2 MASS MIXING RATIO AFTER TIMESTEP
 help=Hydrogen Mass Mixing Ratio in kg/kg(Air)
@@ -18069,6 +18077,16 @@
 description=O3P MASS MIXING RATIO ON PRESS LEVS
 help=Oxygen atom (ground state) Mass Mixing Ratio in kg/kg(Air)
 
+[stashmaster:code(51064)]
+description=ALICE MASS MIXING RATIO AFTER TIMESTEP
+help=UKCA Tutiorial Tracer ALICE Mass Mixing Ratio in kg/kg(Air)
+    =on pressure levels
+
+[stashmaster:code(51065)]
+description=BOB MASS MIXING RATIO AFTER TIMESTEP
+help=UKCA Tutiorial Tracer BOB Mass Mixing Ratio in kg/kg(Air)
+    =on pressure levels
+
 [stashmaster:code(51070)]
 description=H2 MASS MIXING RATIO ON PRESS LEVS
 help=Hydrogen Mass Mixing Ratio in kg/kg(Air)
Index: rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A
===================================================================
--- rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A (revision 30974)
+++ rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A (revision 30979)
@@ -13933,6 +13933,18 @@
 4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
 5|    0 | 2160 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
 #
+1|    1 |   34 |   64 |ALICE  MASS MIXING RATIO AFTER TS   |
+2|    2 |    0 |    1 |    1 |    2 |   40 |   11 |    0 |    0 |    0 |    0 |
+3| 000000000000000000000000010000 | 00000000000000000001 |    1 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 2164 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   34 |   65 |BOB    MASS MIXING RATIO AFTER TS   |
+2|    2 |    0 |    1 |    1 |    2 |   40 |   11 |    0 |    0 |    0 |    0 |
+3| 000000000000000000000000010000 | 00000000000000000001 |    1 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 2165 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
+#
 1|    1 |   34 |   69 |CH3OH MASS MIXING RATIO AFTER TS    |
 2|    2 |    0 |    1 |    1 |    2 |   40 |   11 |    0 |    0 |    0 |    0 |
 3| 000000000000000000000000000100 | 00000000000000000001 |    1 |
@@ -21785,6 +21797,18 @@
 4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
 5|    0 | 2160 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
 #
+1|    1 |   51 |   64 |ALICE  MASS MIX RATIO ON PRESS LEVS |
+2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
+3| 000000000000000000000000010000 | 00000000000000000001 |    3 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 2164 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   51 |   65 |BOB    MASS MIX RATIO ON PRESS LEVS |
+2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
+3| 000000000000000000000000010000 | 00000000000000000001 |    3 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 2165 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
+#
 1|    1 |   51 |   69 |CH3OH MASS MIX RATIO ON PRESS LEVS  |
 2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
 3| 000000000000000000000000000100 | 00000000000000000001 |    3 |
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task4.1/task4.1.rose.diff** on PUMA.

If you open the **.pk** file in Xconv, you should see the following fields:

```
0    : 192   144   36    1     O3 MASS MIXING RATIO
1    : 192   144   36    1     Molar flux density
2    : 192   144   85    1     O3 MASS MIXING RATIO
3    : 192   144   85    1     Field code =  2164
4    : 192   144   85    1     Field code =  2165
```

Sample output from this task can be found at **/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task4.1/ai084a.pk19880901** on ARCHER.

Tutorial 5

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 5

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

During this tutorial you will learn how to make new UKCA netCDF emissions files. Then you will learn how to add new emissions into UKCA so that they emit into one of your new tracers.

At the end of the previous tutorial you will now know how to create new tracers for use by UKCA. However, after completing the tasks, your tracers will still be empty, as nothing has been put into them. This tutorial will teach you how to create an emissions file that the UKCA will read, and that you can then tell UKCA to use and emit into your tracer(s).

This tutorial will go through the steps needed to make an emission into a tracer which UKCA does not currently emit into. The steps in making the netCDF file will be the same for a species which is currently emitted into, although in this simpler case you would not need to make any code changes.

Task 5.1: Create a new emissions file and use it in your job

Task 5.1: In the

```
/work/n02/n02/ukca/Tutorial/vn10.4/Task5.1
```

directory on ARCHER there is the file **Emissions_of_ALICE.nc** which is a 0.5x0.5 degree resolution surface emission field. You should regrid this file to the **N96 ENDGame grid**, and output it as a netCDF file that has the required netCDF metadata for a climatological surface emission without any diurnal cycle.

The netCDF emissions system

UKCA uses netCDF files to specify the emissions into UKCA species. Using netCDF files means that the **metadata** in the file can be used to specify various options, such as which diurnal cycle to use.

Metadata

In Global Atmosphere 7.0, UKCA emissions are prescribed using netCDF files. The reason for this move away from the UM ancillary file format

Each emission field in the NetCDF files needs to include the following variable metadata attributes (there is no requirement for the netCDF variable names themselves except that they be no longer than 80 characters):

- **`standard_name`:** It should be included if an appropriate name is present in the CF Standard Name Table (see http://cfconventions.org/standard-names.html). An example of a valid ‘standard name’ is:

  `“tendency_of_atmosphere_mass_content_of_nitrogen_monoxide_due_to_emission”`

  (note that all substrings have to be separated by underscores).

- **`long_name`:** It is recommendable but only compulsory if there is no ‘standard_name’ available for that emission field. There are no specific CF conventions for standard names, but within the UKCA code all substrings should be separated by white space as shown in this example:

  `“tendency of atmosphere mass content of nitrogen monoxide due to emission”.`

  The reason for this is given in the description of the attribute units.

- **`tracer_name`:** This attribute has to be equal to the name of a tracer (or of an emission field such as ‘NO - aircrft’) present in the list of emissions for the given chemical scheme, i.e. `em_chem_spec`. This name is used by the subroutine UKCA_ADD_EMISS to add the emission field to the corresponding tracer. There should be at least one emission field in the NetCDF files (or alternatively an online emission field) with the value of tracer name equal to one of the items in em_chem_spec, otherwise the subroutine UKCA_EMISS_INIT (in module UKCA_EMISS_MOD) will report a missing tracer in the emission files and the model will stop with error.
- **`units`:** According to CF conventions, all emissions should be expressed in $kg\, m^{-2}\, s^{-1}$. As a consequence, all files will contain the attribute

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

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

- **`hourly_scaling`: (optional)** A character attribute used to apply a diurnal cycle to emissions data with daily or lower frequency. Allowed values:
    - `none` (or attribute not present): no scaling
    - `traffic_uk`: used for UK air quality studies
    - `TNO_MACC_EU_SNAPnn` (where nn=01 to 11): Hourly factors of emissions for Europe. Calculated by TNO for the MACC project.
    - `diurnal_isopems` (for isoprene emissions): use the routine UKCA DIURNAL ISOP EMS to calculate a diurnal cycle using solar zenith angle and latitude to compute the expected number of sunshine hours.
- **`daily_scaling` (optional):** A character attribute used to apply a weekly cycle to emissions weekly or lower frequency. Only allowed when the model is using the Gregorian calendar. Allowed values:
    - `none` (or attribute not present): no scaling
    - `traffic_uk`: used for UK air quality studies
    - `TNO_MACC_GB_SNAPnn` (where nn=01 to 11): Hourly factors of emissions for Great Britain. Calculated by TNO for the MACC project.
- **`vertical_scaling` (optional):** A character attribute defining the vertical distribution of the emission. This allows the user to supply a 2D field to be applied over multiple levels. Allowed values:
    - `surface` (or attribute not present): treat as surface emission
    - `all_levels`, `3D`: field is three-dimensional and is provided on model levels (must have the same number of levels as the model)
    - `high_level`: spread a 2D field over multiple model levels, weighting by model layer thickness to achieve a uniform distribution in height. Must be accompanied by variable attributes lowest level and highest level to indicate the model levels over which to distribute the emission.
    - `step1`: used for air quality simulations, spreads emission over lowest 3 layers of the model; only allowed with 38 model levels.
    - `EMEP_modified_SNAPnn` (where nn=01 to 11): Average vertical profiles for SNAP sectors, similar to implementation for EMEP model. See routine vertical emiss factors for details.
    - `Bieser_modified_SNAPnn` (where nn=01 to 11): Average vertical profiles for SNAP sectors, similar to implementation of Bieser et al. (2011) with the SMOKE model and including fugitive emissions. See routine vertical_emiss_factors for details. In addition, each NetCDF file has to include two global attributes with information that is valid for all emission fields present in the file:
- **`update_freq_in_hours`:** Integer indicating the frequency (in hours) at which all emission fields present in that file should be read to update emissions(:)%values (:,:,:) in the UKCA code. Update points are calculated relative the model’s ancil reftime.
- **`update_type`**: Integer number indicating the times at which the data is provided. The same conventions as for ancillary files have been adopted:
    - 0: Single time
    - 1: Time series
    - 2: Periodic time series

When emissions are treated as time series (update_type=1) the user is responsible for creating emission fields which cover the whole period for which the model is run; otherwise the model will not find the time registers to do interpolations and will stop with error. When emissions are periodic (update_type=2) each emission field has to include exactly 12 monthly average emissions (Jan, Feb, ..., Dec). Other attributes, in particular some global attributes, as well as some additional fields (e.g. a variable indicating the type of grid mapping) should be present in the files to comply with CF conventions for NetCDF data, but they are not used by the UKCA code.

Using python to regrid your emissions

For this task we will be using the Iris (http://scitools.org.uk/iris/) python library, which is developed by the Met Office and can read Met Office formatted files. The cf-python (http://cfpython.bitbucket.org/) library also does this, but we will not be using this here.

You can use Iris on ARCHER by loading the anaconda (https://www.continuum.io/anaconda-overview) module:

```
module load anaconda
```

if you then

```
conda list
```

you will see that Iris is available:

```
iris                      1.10.0               np19py27_2    https://conda.binstar.org/scitools
```

when developing python scripts, a good command to use can be set by the following alias:

```
alias pylab='ipython --pylab --logfile=ipython-`date +"%Y%m%d-%H%M%S"`.py'
```

This uses ipython (http://ipython.readthedocs.io/en/stable/) , which is an interactive shell for python. The `--pylab` automatically loads some standard python libraries such as scipy (https://www.scipy.org/) , numpy (http://www.numpy.org/) , and matplotlib (http://matplotlib.org/) . The `--logfile` means that all commands will be recorded in a file with the format `ipython-YYYYMMDD-HHMMSS.py`.

You can also execute pre-written python scripts by

```
python2.7 -c "execfile('name_of_script.py')"
```

However, **don't panic**. **You are not expected to know python to complete this tutorial.** You will be provided with an example script to use that you only need to edit a few lines to get to work. You do not need to write a script from scratch, just read-through the provided script and try to understand what it does, and why.

Example python script

In the directory:

```
/work/n02/n02/ukca/Tutorial/vn10.4/Task5.1
```

you will find the file **`regrid_ALICE_N96e.py`**. You should take a copy of this file, and using your output **.pk** file from your suite, you should regrid the emissions into the N96 ENDGame grid. You will later use the resulting netCDF file in your suite.

This file looks like:

```
#!/usr/bin/env python

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4

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# Written by N. Luke Abraham 2016-10-20 <nla27@cam.ac.uk>

# preamble
import iris
import numpy
# pre-Iris v1.10, use iris.unit instead of cf_units
import cf_units

# --- CHANGE THINGS BELOW THIS LINE TO WORK WITH YOUR FILES ETC. ---

# name of file containing an ENDGame grid, e.g. your model output
# NOTE: all the fields in the file should be on the same horizontal
#       grid, as the field used MAY NOT be the first in order of STASH
grid_file='ai084a.pk19880901'
# name of emissions file
emissions_file='Emissions_of_ALICE.nc'

# --- BELOW THIS LINE, NOTHING SHOULD NEED TO BE CHANGED ---

species_name='ALICE'

# this is the grid we want to regrid to, e.g. N96 ENDGame
grd=iris.load(grid_file)[0]
grd.coord(axis='x').guess_bounds()
grd.coord(axis='y').guess_bounds()

# This is the original data
ems=iris.load_cube(emissions_file)
# make intersection between 0 and 360 longitude to ensure that
# the data is regridded correctly
nems = ems.intersection(longitude=(0, 360))

# make sure that we use the same coordinate system, otherwise regrid won't work
nems.coord(axis='x').coord_system=grd.coord_system()
nems.coord(axis='y').coord_system=grd.coord_system()

# now guess the bounds of the new grid prior to regridding
nems.coord(axis='x').guess_bounds()
nems.coord(axis='y').guess_bounds()

# now regrid
ocube=nems.regrid(grd,iris.analysis.AreaWeighted())

# now add correct attributes and names to netCDF file
ocube.var_name='emissions_'+str.strip(species_name)
ocube.long_name=str.strip(species_name)+' surf emissions'
ocube.units=cf_units.Unit('kg m-2 s-1')
ocube.attributes['vertical_scaling']='surface'
ocube.attributes['tracer_name']=str.strip(species_name)
```
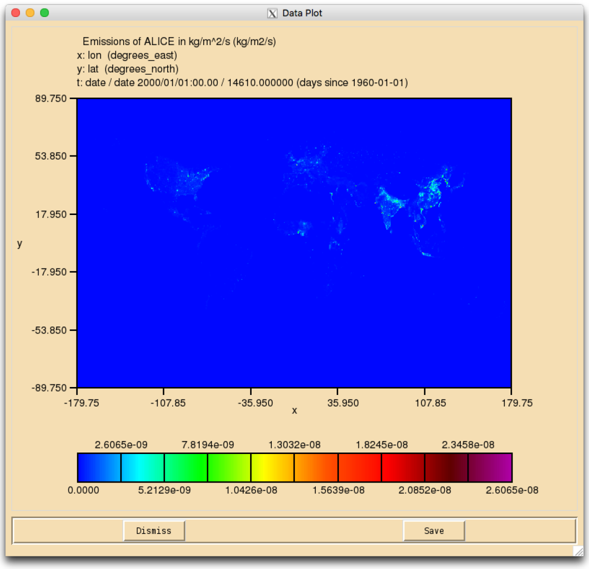
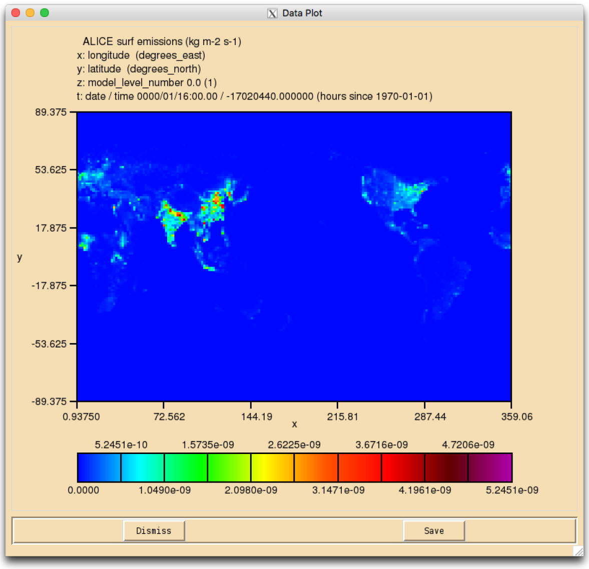

```
# global attributes, so don't set in local_keys
# NOTE: all these should be strings, including the numbers! This will change at a later UM version.
# basic emissions type
ocube.attributes['emission_type']='2' # periodic
ocube.attributes['update_type']='2'   # same as above
ocube.attributes['update_freq_in_hours']='120' # i.e. 5 days
ocube.attributes['source']='UKCA Tutorial Task 5.1 - creating netCDF emissions'

# rename and set time coord - set to be 0000/01/16:00:00-0000/12/16:00:00
# this bit is annoyingly fiddly
ocube.coord(axis='t').var_name='time'
ocube.coord(axis='t').standard_name='time'
ocube.coords(axis='t')[0].units=cf_units.Unit('hours since 1970-01-01', calendar='360_day')
ocube.coord(axis='t').points=numpy.array([-17020440, -17019720, -17019000, -17018280,
                                          -17017560, -17016840, -17016120, -17015400,
                                          -17014680, -17013960, -17013240, -17012520])
# make z-direction.
zdims=iris.coords.DimCoord(numpy.array([0]),standard_name = 'model_level_number',
                           units='1',attributes={'positive':'up'})
ocube.add_aux_coord(zdims)
ocube=iris.util.new_axis(ocube, zdims)
# now transpose cube to put Z 2nd
ocube.transpose([1,0,2,3])

# make coordinates 64-bit
ocube.coord(axis='x').points=ocube.coord(axis='x').points.astype(dtype='float64')
ocube.coord(axis='y').points=ocube.coord(axis='y').points.astype(dtype='float64')
#ocube.coord(axis='z').points=ocube.coord(axis='z').points.astype(dtype='float64') # integer
ocube.coord(axis='t').points=ocube.coord(axis='t').points.astype(dtype='float64')
# for some reason, longitude_bounds are double, but latitude_bounds are float
ocube.coord('latitude').bounds=ocube.coord('latitude').bounds.astype(dtype='float64')


# add forecast_period & forecast_reference_time
# forecast_reference_time
frt=numpy.array([-17020080, -17019360, -17018640, -17017920,
                 -17017200, -17016480, -17015760, -17015040,
                 -17014320, -17013600, -17012880, -17012160],dtype='float64')
frt_dims=iris.coords.AuxCoord(frt,standard_name = 'forecast_reference_time',
                           units=cf_units.Unit('hours since 1970-01-01', calendar='360_day'))
ocube.add_aux_coord(frt_dims,data_dims=0)
ocube.coord('forecast_reference_time').guess_bounds()
# forecast_period
fp=numpy.array([-360],dtype='float64')
fp_dims=iris.coords.AuxCoord(fp,standard_name = 'forecast_period',
                           units=cf_units.Unit('hours'),bounds=numpy.array([-720,0],dtype='float64'))
ocube.add_aux_coord(fp_dims,data_dims=None)

# add-in cell_methods
ocube.cell_methods = [iris.coords.CellMethod('mean', 'time')]
# set _FillValue
fillval=1e+20
ocube.data = numpy.ma.array(data=ocube.data, fill_value=fillval, dtype='float32')

# output file name, based on species
outpath='ukca_emiss_'+species_name+'.nc'
# don't want time to be cattable, as is a periodic emissions file
iris.FUTURE.netcdf_no_unlimited=True
# annoying hack to set a missing_value attribute as well as a _FillValue attribute
dict.__setitem__(ocube.attributes, 'missing_value', fillval)
# now write-out to netCDF
saver = iris.fileformats.netcdf.Saver(filename=outpath, netcdf_format='NETCDF3_CLASSIC')
saver.update_global_attributes(Conventions=iris.fileformats.netcdf.CF_CONVENTIONS_VERSION)
saver.write(ocube, local_keys=['vertical_scaling', 'missing_value','um_stash_source','tracer_name'])

# end of script

# Why we are messing around with metadata?
#-----------------------------------------
#
# We need to adapt the metadata of the emissions data to
# match what UKCA is expecting.
#  e.g. the metadata of the 'Emissions_of_ALICE.nc file is:
#
#    netcdf Emissions_of_ALICE {
#    dimensions:
#            lon = 720 ;
#            lat = 360 ;
#            date = UNLIMITED ; // (12 currently)
#    variables:
```

```
#            float lon(lon) ;
#                    lon:long_name = "Longitude" ;
#                    lon:standard_name = "longitude" ;
#                    lon:units = "degrees_east" ;
#                    lon:point_spacing = "even" ;
#                    lon:modulo = " " ;
#            float lat(lat) ;
#                    lat:long_name = "Latitude" ;
#                    lat:standard_name = "latitude" ;
#                    lat:units = "degrees_north" ;
#                    lat:point_spacing = "even" ;
#            float date(date) ;
#                    date:long_name = "Time" ;
#                    date:units = "days since 1960-01-01" ;
#                    date:time_origin = "01-JAN-1960:00:00:00" ;
#            float ALICE(date, lat, lon) ;
#                    ALICE:source = " " ;
#                    ALICE:name = "ALICE" ;
#                    ALICE:title = "Emissions of ALICE in kg/m^2/s" ;
#                    ALICE:date = "01/01/60" ;
#                    ALICE:time = "00:00" ;
#                    ALICE:long_name = "Emissions of ALICE in kg/m^2/s" ;
#                    ALICE:standard_name = "tendency_of_atmosphere_mass_content_of_ALICE_due_to_emission" ;
#                    ALICE:units = "kg/m2/s" ;
#                    ALICE:missing_value = 2.e+20f ;
#                    ALICE:_FillValue = 2.e+20f ;
#                    ALICE:valid_min = 0.f ;
#                    ALICE:valid_max = 2.60646e-08f ;
#
#    // global attributes:
#                    :history = "Tue Jun 18 14:32:42 BST 2013 - XCONV V1.92 16-February-2006" ;
#    }
#
#  whereas, the metadata of the
#  /work/n02/n02/hum/ancil/atmos/n96e/ukca_emiss/cmip5/2000/v2/ukca_emiss_CO.nc
#  file is, e.g.:
#
#    netcdf ukca_emiss_CO {
#    dimensions:
#            time = UNLIMITED ; // (12 currently)
#            model_level_number = 1 ;
#            latitude = 144 ;
#            longitude = 192 ;
#            bnds = 2 ;
#    variables:
#            double emissions_CO(time, model_level_number, latitude, longitude) ;
#                    emissions_CO:long_name = "CO surf emissions" ;
#                    emissions_CO:units = "kg m-2 s-1" ;
#                    emissions_CO:um_stash_source = "m01s00i303" ;
#                    emissions_CO:tracer_name = "CO" ;
#                    emissions_CO:vertical_scaling = "surface" ;
#                    emissions_CO:cell_methods = "time: mean" ;
#                    emissions_CO:grid_mapping = "latitude_longitude" ;
#                    emissions_CO: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:bounds = "time_bnds" ;
#                    time:units = "hours since 1970-01-01 00:00:00" ;
#                    time:standard_name = "time" ;
#                    time:calendar = "360_day" ;
#            double time_bnds(time, bnds) ;
#            int model_level_number(model_level_number) ;
#                    model_level_number:axis = "Z" ;
#                    model_level_number:units = "metre" ;
#                    model_level_number:standard_name = "model_level_number" ;
#                    model_level_number:long_name = "height at theta layer midpoint" ;
#                    model_level_number:positive = "up" ;
#            float latitude(latitude) ;
#                    latitude:axis = "Y" ;
#                    latitude:bounds = "latitude_bnds" ;
#                    latitude:units = "degrees_north" ;
#                    latitude:standard_name = "latitude" ;
#            float latitude_bnds(latitude, bnds) ;
#            float longitude(longitude) ;
#                    longitude:axis = "X" ;
#                    longitude:bounds = "longitude_bnds" ;
#                    longitude:units = "degrees_east" ;
#                    longitude:standard_name = "longitude" ;
#            double longitude_bnds(longitude, bnds) ;
#            double forecast_period ;
#                    forecast_period:bounds = "forecast_period_bnds" ;
#                    forecast_period:units = "hours" ;
#                    forecast_period:standard_name = "forecast_period" ;
#            double forecast_period_bnds(bnds) ;
#            double forecast_reference_time(time) ;
#                    forecast_reference_time:units = "hours since 1970-01-01 00:00:00" ;
#                    forecast_reference_time:standard_name = "forecast_reference_time" ;
#                    forecast_reference_time:calendar = "360_day" ;
#
#    // global attributes:
#                    :emission_type = "2" ;
#                    :source = "Data from Met Office Unified Model" ;
#                    :um_version = "7.3" ;
#                    :update_freq_in_hours = "120" ;
#                    :update_type = "2" ;
#                    :Conventions = "CF-1.5" ;
#    }
#
#  so the metadata of our new emissions file needs to be edited to be what UKCA
#  expects.
#
#  After using this script, the resultant netCDF file should look like:
#
#    netcdf ukca_emiss_ALICE {
#    dimensions:
#            time = 12 ;
#            model_level_number = 1 ;
#            latitude = 144 ;
#            longitude = 192 ;
#            bnds = 2 ;
#    variables:
#            float emissions_ALICE(time, model_level_number, latitude, longitude) ;
#                    emissions_ALICE:_FillValue = 1.e+20f ;
#                    emissions_ALICE:long_name = "ALICE surf emissions" ;
#                    emissions_ALICE:units = "kg m-2 s-1" ;
#                    emissions_ALICE:missing_value = 1.e+20f ;
#                    emissions_ALICE:tracer_name = "ALICE" ;
#                    emissions_ALICE:vertical_scaling = "surface" ;
#                    emissions_ALICE:cell_methods = "time: mean" ;
#                    emissions_ALICE:grid_mapping = "latitude_longitude" ;
#                    emissions_ALICE: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 = "hours since 1970-01-01" ;
#                    time:standard_name = "time" ;
#                    time:long_name = "Time" ;
#                    time:calendar = "360_day" ;
#                    time:time_origin = "01-JAN-1960:00:00:00" ;
#            int model_level_number(model_level_number) ;
#                    model_level_number:axis = "Z" ;
#                    model_level_number:units = "1" ;
#                    model_level_number:standard_name = "model_level_number" ;
#                    model_level_number:positive = "up" ;
#            double latitude(latitude) ;
#                    latitude:axis = "Y" ;
#                    latitude:bounds = "latitude_bnds" ;
#                    latitude:units = "degrees_north" ;
#                    latitude:standard_name = "latitude" ;
#            double latitude_bnds(latitude, bnds) ;
#            double longitude(longitude) ;
#                    longitude:axis = "X" ;
#                    longitude:bounds = "longitude_bnds" ;
#                    longitude:units = "degrees_east" ;
#                    longitude:standard_name = "longitude" ;
#            double longitude_bnds(longitude, bnds) ;
#            double forecast_period ;
#                    forecast_period:bounds = "forecast_period_bnds" ;
#                    forecast_period:units = "hours" ;
#                    forecast_period:standard_name = "forecast_period" ;
#            double forecast_period_bnds(bnds) ;
#            double forecast_reference_time(time) ;
#                    forecast_reference_time:bounds = "forecast_reference_time_bnds" ;
#                   forecast_reference_time:units = "hours since 1970-01-01" ;
#                   forecast_reference_time:standard_name = "forecast_reference_time" ;
#                   forecast_reference_time:calendar = "360_day" ;
#           double forecast_reference_time_bnds(time, bnds) ;
#
#    // global attributes:
#                   :Conventions = "CF-1.5" ;
#                   :date = "01/01/60" ;
#                   :emission_type = "2" ;
#                   :history = "Tue Jun 18 14:32:42 BST 2013 - XCONV V1.92 16-February-2006" ;
#                   :invalid_standard_name = "tendency_of_atmosphere_mass_content_of_ALICE_due_to_emission" ;
#                   :name = "ALICE" ;
#                   :source = "UKCA Tutorial Task 5.1 - creating netCDF emissions" ;
#                   :time = "00:00" ;
#                   :title = "Emissions of ALICE in kg/m^2/s" ;
#                   :update_freq_in_hours = "120" ;
#                   :update_type = "2" ;
#    }
```

Solution to Task5.1



ALICE emissions prior to regridding.



ALICE emissions after regridding. Note the shift of the grid.

A file that has been produced by the above script can be found at

```
/work/n02/n02/ukca/Tutorial/vn10.4/Task5.1/solution/ukca_emiss_ALICE.nc
```

Task 5.2: make the required code changes to add your emission into UKCA

TASK 5.2: You should now make the UKCA code changes to add your emission into the **ALICE** tracer.

Hint [hide]
You will need to add-in the molar mass of ALICE. You can calculate this from the mass of air and the conversion factor defined in Task 4.1.

Rose changes

To include this netCDF file, you should go to the UKCA panel and scroll down until you find the settings for `ukca_em_files`. Click the **blue plus symbol** to add an extra line, and put the full path to the new file. On ARCHER, this file will need to be on `/work` as the batch queues are unable to see `/home`.

Code changes

`ukca_chem_strattrop.F90`

You can choose to put a **1** in the **E** column of the `chch_defs_scheme_chem/aer` arrays. This is just for completeness however, as this column is not currently used.

`ukca_setd1defs.F90`

You will need to edit the **`em_chem_spec`** array for the scheme that you are using to include the new species that you are emitting into. By convention, these are ordered as 2D fields followed by 3D fields. If the tracer is valid for both with and without aerosol chemistry (& GLOMAP) you will need to put this in twice.

`ukca_constants.F90`

You will need to define the **`M_species`** for the emitted species. This should be consistent with the **`C_species`** value set in the previous tutorial.

`get_molmass_mod.F90`

You will need to add to the **`species_name`** `CASE` statement, to include a line such as this

```
CASE ('ALICE     ')
  get_molmass = m_ALICE
```

for each new species that you are emitting into.

Solution to Task 5.2

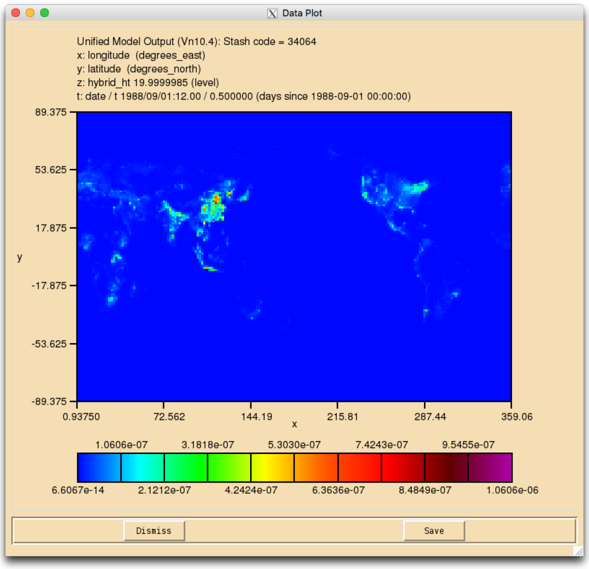


Figure 1: Surface level concentrations (kg/kg) of ALICE after emissions have been applied.

You were given the task

- *In the*

  ```
  /work/n02/n02/ukca/Tutorial/vn10.4/Task5.1
  ```

  *directory on ARCHER there is the file **Emissions_of_ALICE.nc** which is a 0.5x0.5 degree resolution surface emission field. You should regrid this file to the **N96 ENDGame grid**, and output it as a netCDF file that has the required netCDF metadata for a climatological surface emission without any diurnal cycle.*

You were given the hint

- *You will need to add-in the molar mass of ALICE. You can calculate this from the mass of air and the conversion factor defined in Task 4.1.*

For a working Rose suite that has completed this task, please see **`u-ai084@25943`**

The specific Rose changes made are:

```
Index: trunk/app/um/rose-app.conf
=================================================================
--- trunk/app/um/rose-app.conf  (revision 25815)
+++ trunk/app/um/rose-app.conf  (revision 25943)
@@ -4073,7 +4073,8 @@
              ='$UM_NETCDF_UKCAEMISS_MECHO_DIR/$UM_NETCDF_UKCA
              ='$UM_NETCDF_UKCAEMISS_ME2CO_DIR/$UM_NETCDF_UKCA
              ='$UM_NETCDF_UKCAEMISS_NH3_DIR/$UM_NETCDF_UKCAEM
-             ='$UM_NETCDF_UKCAEMISS_NOAIR_DIR/$UM_NETCDF_UKCA
+             ='$UM_NETCDF_UKCAEMISS_NOAIR_DIR/$UM_NETCDF_UKCA
+             ='/work/n02/n02/ukca/Tutorial/vn10.4/Task5.1/sol
 ukca_h1202mmr=3.788e-13
 ukca_h1211mmr=2.225e-11
 ukca_h1301mmr=1.363e-11
Index: trunk/app/fcm_make_um/rose-app.conf
=================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 25815)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 25943)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox
```

These differences can be found in the file **`/home/ukca/Tutorial/worked_solutions/Task5.2/task5.2.rose.diff`** on PUMA.

For a working UM branch that has completed this task, please see **`fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@31082`**

The specific UM changes made are:

```
Index: src/atmosphere/UKCA/ukca_setd1defs.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setd1defs.F90      (revision 30979)
+++ src/atmosphere/UKCA/ukca_setd1defs.F90      (revision 31082)
@@ -301,7 +301,7 @@
       nr_phot         = 38
     END IF
   ELSE IF (L_ukca_strattrop .AND. .NOT. L_ukca_achem) THEN
```

```
-    n_chem_emissions = 9
+    n_chem_emissions = 10
     n_3d_emissions = 1       ! aircraft NOX
     n_aero_tracers =  0
     ALLOCATE(em_chem_spec(n_chem_emissions+n_3d_emissions))
@@ -308,19 +308,20 @@
     em_chem_spec =                                            &
         (/'NO        ','CH4       ','CO        ','HCHO      ', &
           'C2H6      ','C3H8      ','Me2CO     ','MeCHO     ', &
-          'C5H8      ','NO_aircrft'/)
+          'C5H8      ','ALICE     ','NO_aircrft'/)
     n_chem_tracers = 73         ! No chem tracers
     nr_therm       = 220        ! thermal reactions
     nr_phot        = 55         ! photolytic (ATA)

   ELSE IF (L_ukca_strattrop .AND. L_ukca_achem) THEN
-    n_chem_emissions = 19      ! em_chem_spec below
+    n_chem_emissions = 20      ! em_chem_spec below
     n_3d_emissions   = 4       ! BC, OC, 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 ', &
+          'C5H8      ','ALICE     ',                           &
+          'BC_fossil ','BC_biofuel','OC_fossil ',              &
          'OC_biofuel','Monoterp  ','NVOC      ','SO2_low   ', &
          'SO2_high  ','NH3       ','DMS       ','SO2_nat   ', &
          'BC_biomass','OC_biomass','NO_aircrft'/)
Index: src/atmosphere/UKCA/get_molmass_mod.F90
===================================================================
--- src/atmosphere/UKCA/get_molmass_mod.F90     (revision 30979)
+++ src/atmosphere/UKCA/get_molmass_mod.F90     (revision 31082)
@@ -243,6 +243,11 @@
   get_molmass = m_brcl

   ! ----------------------------------------
+  !   UKCA Tutorial Tracer
+CASE ('ALICE     ')
+  get_molmass = m_ALICE
+
+  ! ----------------------------------------
   !   Others (report warning)
 CASE ('AGE       ')
   get_molmass =  1.0
Index: src/atmosphere/UKCA/ukca_constants.F90
===================================================================
--- src/atmosphere/UKCA/ukca_constants.F90      (revision 30979)
+++ src/atmosphere/UKCA/ukca_constants.F90      (revision 31082)
@@ -390,6 +390,9 @@
 REAL, PARAMETER :: m_aromooh  = 130.0
 REAL, PARAMETER :: m_mekooh   = 104.0

+!     UKCA Tutorial tracers - only ALICE is emitted
+REAL, PARAMETER :: m_ALICE    = 28.97
+
 !     The mass of organic nitrate is an approximation,
 !     calculated as the average of ORGNIT formed by two
 !     reacs. in UKCA_CHEMCO_RAQ:
Index: src/atmosphere/UKCA/ukca_chem_strattrop.F90
===================================================================
--- src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 30979)
+++ src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31082)
@@ -215,7 +215,7 @@
 !  75
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  76
-chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  0),  &
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  1),  &
 !  77
 chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0)   &
  /)
@@ -372,7 +372,7 @@
 !  75
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  76
-chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  0),  &
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  1),  &
 !  77
```

```
chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0),  &
!  78
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task5.2/task5.2.um.diff** on PUMA.

If you open the **.pk** file in Xconv, you should still see the following fields:

```
0    : 192   144   36    1     O3 MASS MIXING RATIO
1    : 192   144   36    1     Molar flux density
2    : 192   144   85    1     O3 MASS MIXING RATIO
3    : 192   144   85    1     Field code =  2164
4    : 192   144   85    1     Field code =  2165
```

Sample output from this task can be found at **/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task5.2/ai084a.pk19880901** on ARCHER.

Tutorial 6

Written by Luke Abraham 2016. Many thanks to Alistair Sellar for the notes on netCDF metadata.

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UKCA Chemistry and Aerosol vn10.4 Tutorial 6

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this tutorial

During this tutorial you will learn how UKCA specifies different chemical reactions. You will then add a new reaction involving the new tracers that you have added.

Task 6.1: Add a bimolecular reaction

TASK 6.1: You should now add in the bimolecular reaction of **ALICE** with **OH** to form **BOB** and a ***secondary organic compound*** (labelled in UKCA as **Sec_Org**). This reaction is given by:

$$\mathrm{ALICE} + \mathrm{OH} \longrightarrow \mathrm{BOB} + \mathrm{Sec\_Org}$$

Parameter	Value
k_0	2.70E-11
α	0.00
β	-390.00

Adding new Chemical Reactions

UKCA currently uses two different methods of defining the chemical reactions solved in the model. The first is a backward Euler solver, and is used for the *RAQ* and *StdTrop* chemistry schemes where the solver itself is created by a code-writer. The second makes use of the ASAD chemical integration software package (http://www.atm.ch.cam.ac.uk/acmsu/asad/) , and is used for the *CheT/TropIsop*, *CheS/Strat*, and *CheST/StratTrop* chemistry schemes. ASAD can use many different solvers, although currently it uses a symbolic Newton-Raphson solver. In this tutorial we will only consider the ASAD framework, as this is easily extended by a user.

ASAD considers four different types of chemical reactions: bimolecular reactions, termolecular reactions, heterogeneous reactions, and photolysis reactions. To make changes and add reactions you will need to make changes to the UKCA source code which can be found in

```
vn10.4_your_branch_name/src/atmosphere/UKCA
```

During this tutorial you will be tasked with adding a new reaction into your branch.

Biomolecular Reactions

For most bimolecular reactions, it is sufficient to provide the k_0, α, and β coefficients that are used to compute the rate coefficient k from the Arrhenius expression

$$k = k_0 \left(\frac{T}{300}\right)^{\alpha} \exp\left(\frac{-\beta}{T}\right)$$

Bimolecular Reaction Definition

The bimolecular reactions are defined in the **ukca_chem_scheme.F90** routines using the **ratb_t** Fortran type specification, and are held in arrays. At the end of this routine the **ratb_defs_scheme** array is created from these, and if that scheme is selected in UKCA these reactions are copied across into the master **ratb_defs** array.

The format of this **ratb_t** type is

```
ratb_t('Reactant 1','Reactant 2','Product 1 ','Product 2 ','Product 3 ',&
'Product 4 ', k0, α, β, Fraction of Product 1 produced, Fraction of Product 2 produced, Fraction of Product 3
```

If fractional products are not required for a reaction, then the *fraction of each product* formed should be set to 0.000. If fractional products are required for any one of the products then the fraction of each product formed should be set to its correct value.

The specifications of the individual reactions are done as, e.g.

```
ratb_t('O3        ','C5H8      ','HO2       ','OH        ','          ',& ! B133
'          ',  3.33E-15,  0.00,   1995.00, 0.750, 0.750, 0.000, 0.000), & ! B133 IUPAC2007*
...
ratb_t('OH        ','C5H8      ','ISO2      ','          ','          ',& ! B144
'          ',  2.70E-11,  0.00,   -390.00, 0.000, 0.000, 0.000, 0.000), & ! B144 IUPAC2009
...
ratb_t('OH        ','HCl       ','H2O       ','Cl        ','          ',& ! B159
'          ',  1.80E-12,  0.00,    250.00, 0.000, 0.000, 0.000, 0.000), & ! B159 JPL2011
```

The first reaction in these examples takes its kinetic data from IUPAC (http://www.iupac-kinetic.ch.cam.ac.uk/) . Going to this website, this reaction is defined here (http://www.iupac-kinetic.ch.cam.ac.uk/datasheets/xhtml/HOx_VOC8_HO_CH2C%28CH3%29CHCH2%28isoprene%29.xhtml_mathml.xml) . The second reaction above takes its kinetic data from NASA's Jet Propulsion Laboratory (http://jpldataeval.jpl.nasa.gov/) . The rate for this can be found on page 1-19 of the JPL2011 document (http://jpldataeval.jpl.nasa.gov/pdf/JPL%2010-6%20Final%2015June2011.pdf) . When adding new reactions you will need to increment the size of the array holding the `ratb_t` type.

To add new bimolecular reactions you will need to append equivalent lines for the new reactions to the end of the **ratb_defs_scheme** array (increasing the array sizes accordingly). If there is a reaction that is an exception to the general Arrhenius equation then special code needs to be placed in the **asad_bimol.F90** routine, which is held in the `UKCA/` source-code directory.

Increase the size of JPBK

As well as adding these reactions to the *ukca_chem_scheme.F90* routine (and incrementing the size of the arrays in that routine accordingly, you will also need to increase the value of one parameter that UKCA needs. This is

- **JPBK** is the number of bimolecular reactions

This value is set in `ukca_setup_chem_mod.F90` - you will need to find the correct section of the routine that references the chemistry scheme that you are using, e.g. StratTrop.

Termolecular Reactions

As well as defining reactions involving a third body, the termolecular rate definition can also be used to define unimolecular reactions.

The pressure and temperature dependent rate, k, of a termolecular reaction is given by

$$k = \left(\frac{k_0 [M]}{1 + k_0 [M] / k_\infty} \right) F_c^{\left(1 + \left[\log_{10} \left(\frac{k_0 [M]}{k_\infty} \right) \right]^2 \right)^{-1}}$$

where the low pressure rate constant k_0 is given by

$$k_0 = k_1 \left(\frac{T}{300} \right)^{\alpha_1} \exp \left(\frac{-\beta_1}{T} \right)$$

and the high pressure rate constant k_∞ is given by

$$k_\infty = k_2 \left(\frac{T}{300} \right)^{\alpha_2} \exp \left(\frac{-\beta_2}{T} \right)$$

Termolecular Reaction Definition

The termolecular reactions are defined in the **ukca_chem_scheme.F90** routines using the **ratt_t** Fortran type specification, and are usually held in one single array (there are not usually enough reactions to require splitting the reactions over several arrays).

To format of this **ratt_t** type is

```
ratt_t('Reactant 1','Reactant 2','Product 1 ','Product 2 ', f, &
k1, α1, β1, k2, α2, β2, Fraction of Product 1 produced, Fraction of Product 2 produced), &
```

and as in `ratb_t`, where the fraction of a product should be set to 0.000 if this functionality does not need to be used.

The f value is used to define the F_c value by

If $f < 1.0$ then $F_c = f$

else $F_c = \exp\left(-T/f\right)$

as F_c may or may not be highly temperature dependent.

Examples of these reactions are

```
ratt_t('N2O5      ','m         ','NO2       ','NO3       ',     0.3,     & ! T023
  1.30E-03, -3.50, 11000.00,  9.70E+14,  0.10, 11080.00, 0.000, 0.000), & ! T023 IUPAC 2002
ratt_t('NO        ','NO        ','NO2       ','NO2       ',     0.0,     & ! T024
  3.30E-39,  0.00,  -530.00,  0.00E+00,  0.00,     0.00, 0.000, 0.000)  & ! T024 IUPAC 2001
```

To add new termolecular reactions you will need to append equivalent lines for the new reactions to the end of the **ratt_defs_scheme** array (increasing the array sizes accordingly).

Increase the size of JPTK

As with the bimolecular reactions, you will also need to increase the value of one parameter that UKCA needs. This is

- **JPTK** is the number of termolecular reactions

This value is set in `ukca_setup_chem_mod.F90` - you will need to find the correct section of the routine that references the chemistry scheme that you are using, e.g. StratTrop.

Heterogeneous Reactions

Heterogeneous reactions are those that occur on aerosol surfaces. There is no functional form defined for these reactions, with special code needed to be added for each case.

Heterogeneous Reaction Definition

The heterogeneous reactions are defined in the **ukca_chem_scheme.F90** routines using the **rath_t** Fortran type specification, usually in one array. To format of this **rath_t** type is

```
rath_t('Reactant 1','Reactant 2','Product 1 ','Product 2 ','Product 3 ',&
'Product 4 ', Fraction of Product 1 produced, Fraction of Product 2 produced, Fraction of Product 3 produced, Fr
```

i.e. there is no rate information provided. For reactions on PSCs special code has been added to the routines in **ukca_hetero_mod.F90**, and for other reactions there is code in **asad_hetero.F90**. Examples of this type are

```
rath_t('ClONO2    ','H2O       ','HOCl      ','HONO2     ','          ', &
'          ', 0.000, 0.000, 0.000, 0.000), &
...
rath_t('SO2       ','H2O2      ','NULL0     ','          ','          ', & !HSO3+H2O2(aq)
'          ', 0.000, 0.000, 0.000, 0.000),                                &
```

To add new heterogeneous reactions you will need to append equivalent lines for the new reactions to the end of the **ratt_defs_scheme** array (increasing the array sizes accordingly), before adding code to either **ukca_hetero_mod.F90** or **asad_hetero.F90**.

Increase the size of JPHK

As with the bimolecular and termolecular reactions, you will also need to increase the value of one parameter that UKCA needs. This is

- **JPHK** is the number of heterogeneous reactions

This value is set in `ukca_setup_chem_mod.F90` - you will need to find the correct section of the routine that references the chemistry scheme that you are using, e.g. StratTrop.

Photolysis Reactions

These define a reaction where a chemical compound is broken down by photons. There is no functional form defined for this type of reaction. Instead, either (in the troposphere) input files are used to define the reaction rates for each species, while (in the stratosphere) on-line look-up tables are generated for the rates for each species, or a separate photolysis code, **Fast-JX**, is used to interactively calculate the rate of reaction throughout the the whole atmosphere (for Fast-JX). These interactive schemes are preferred as they take the effect of aerosols or clouds into account at each timestep, allowing for more feedbacks to be investigated. In the upper stratosphere there are some wavelength regions that Fast-JX does not consider, and so the 3D on-line look-up tables are also used for these regions.

Tropospheric Off-Line Photolysis

If Fast-JX is not being used, then the off-line two-dimensional (zonally average) tropospheric photolysis is used (for all schemes). It is based on the work of Hough (1988)[1] and Law *et al* (1998)[2].

This scheme makes use of datafiles which define the reaction rate for a particular species (e.g. H2O2), or if no rate is known, a **nil** rate can be used. For vn10.4 these files can be found in

```
$UMDIR/vn10.4/ctldata/UKCA/tropdata/photol
```

on ARCHER. To use this scheme set the value of `i_ukca_photol` by clicking **2D Photolysis Scheme**. You will then need to give the location of the files (above). The code controlling this scheme is held in **ukca_phot2d.F90**.

It is advised that this scheme is no longer used, and Fast-JX interactive photolysis should be used instead.

References

1. Hough, A. M.: The calculation of photolysis rates for use in global modelling studies, Tech. rep., UK Atomic Energy Authority, Harwell, Oxon., UK, 1988
2. Law, K., Plantevin, P., Shallcross, D., Rogers, H., Pyle, J., Grouhel, C., Thouret, V., and Marenco, A.: Evaluation of modeled O3 using Measurement of Ozone by Airbus In-Service Aircraft (MOZAIC) data, J. Geophys. Res., 103, 25721–25737, 1998

Stratospheric Look-Up Table Photolysis

In a chemistry scheme which has stratospheric chemistry, such as *CheS/Strat* and *CheST/StratTrop*, if interactive photolysis is not used, then above 300hPa the look-up table approach of Lary and Pyle (1991)[1] is used (below 300hPa the tropospheric scheme described above is used). To use this scheme set the value of `i_ukca_photol` by clicking **2D Photolysis Scheme**. The code for this scheme is held in **ukca_strat_update.F90**.

References

1. Lary, D. and Pyle, J.: Diffuse-radiation, twilight, and photochemistry, J. Atmos. Chem., 13, 393–406, 1991.

Interactive Photolysis

The original Fast-J scheme (Wild *et al*, 2000)[1] uses 7 different wavelength bins appropriate for the troposphere, and the updated Fast-JX scheme (Neu et al, 2007)[2] adds up to an extra 11 bins allowing use in the stratosphere. At vn10.4 only Fast-JX is available, although previous UM version used Fast-J as well.

To use this scheme set the value of `i_ukca_photol` by clicking **FastJ-X**. You will then need to give the location of several input data files used by this scheme.

Further details on how the the Fast-JX scheme is used in UKCA, can be found in Telford *et al* (2013) (http://www.geosci-model-dev.net/6/161/2013/gmd-6-161-2013.html) [3].

The Fast-JX data files are held in

```
$UMDIR/vn10.4/ctldata/UKCA/fastj
```

on ARCHER.

References

1. Wild, O., Zhu, X., and Prather, M.: Fast-J: accurate simulation of in- and below-cloud photolysis in tropospheric chemical models, J. Atmos. Chem., 37, 245–282, doi:10.1023/A:1006415919030, 2000
2. Neu, J., Prather, M., and Penner, J.: Global atmospheric chemistry: integrating over fractional cloud cover, J. Geophys. Res., 112, D11306, 12 pp., doi:10.1029/2006JD008007, 2007
3. Telford, P. J., Abraham, N. L., Archibald, A. T., Braesicke, P., Dalvi, M., Morgenstern, O., O'Connor, F. M., Richards, N. A. D., and Pyle, J. A.: Implementation of the Fast-JX Photolysis scheme (v6.4) into the UKCA component of the MetUM chemistry-climate model (v7.3), Geosci. Model Dev., 6, 161-177, doi:10.5194/gmd-6-161-2013, 2013.

Photolysis Reaction Definition

The photolysis reactions are defined in the **ukca_chem_scheme.F90** routines using the **ratj_t** Fortran type specification, usually in several arrays. To format of this **ratj_t** type is

```
ratj_t('Reactant 1','Reactant 2','Product 1 ','Product 2 ','Product 3 ',&
'Product 4 ', Fraction of Product 1 produced, Fraction of Product 2 produced, Fraction of Product 3 produced, Fr
```

The **Look-Up Label** is used to define the file used for the 2D photolysis, and is used by Fast-JX to find the correct values for each species in the input data files. This is a 10-character string, although only the first **7** characters are read by Fast-JX. *Reactant 2* will always be *PHOTON*.

Examples of this type are

```
ratj_t('H2O2      ','PHOTON    ','OH        ','OH        ','          ', &
     '          ',    0.0,   0.0,   0.0,   0.0, 100.000,'jh2o2     ') ,  &
ratj_t('HCHO      ','PHOTON    ','HO2       ','HO2       ','CO        ', &
     '          ',    0.0,   0.0,   0.0,   0.0, 100.000,'jhchoa    ') ,  &
```

Increase the size of JPPJ

As with the bimolecular, termolecular, and heterogeneous reactions, you will also need to increase the value of one parameter that UKCA needs. This is

- **JPPJ** is the number of photolysis reactions

This value is set in `ukca_setup_chem_mod.F90` - you will need to find the correct section of the routine that references the chemistry scheme that you are using, e.g. StratTrop.

Solution to Task 6.1: Add a bimolecular reaction

You were given the task

- *You should now add in the bimolecular reaction of **ALICE** with **OH** to form **BOB** and a* **secondary organic compound** *(labelled in UKCA as **Sec_Org**). This reaction is given by:</span>*

$$\mathrm{ALICE} + \mathrm{OH} \longrightarrow \mathrm{BOB} + \mathrm{Sec\_Org}$$

Parameter	Value
k_0	2.70E-11
α	0.00
β	-390.00

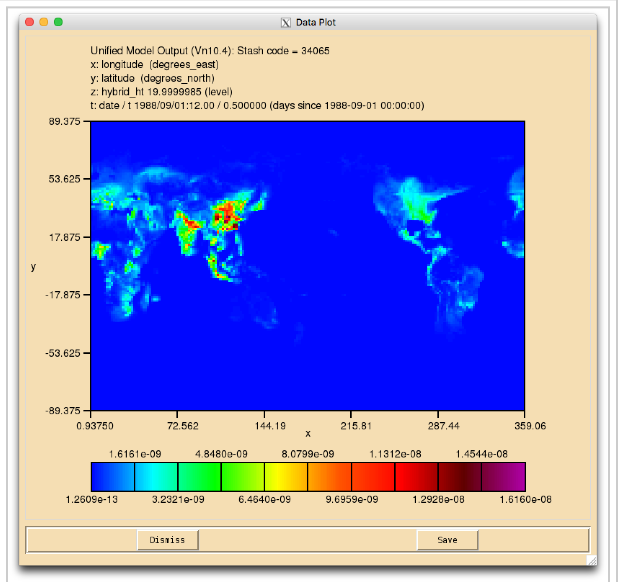

Figure 1: Surface level concentrations (kg/kg) of BOB after the reaction has been applied.

For a working Rose suite that has completed this task, please see **u-ai084@25943**

The specific Rose changes made are (this is just to update the branch revision number):

```
Index: trunk/app/fcm_make_um/rose-app.conf
===================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 25943)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 26542)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task6.1/task6.1.rose.diff** on PUMA.

For a working UM branch that has completed this task, please see **fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@31335**

The specific UM changes made are:

```
Index: src/atmosphere/UKCA/ukca_chem_strattrop.F90
===================================================================
--- src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31082)
+++ src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31335)
@@ -404,7 +404,7 @@
 TYPE(ratb_t) :: ratb_defs_strattrop_chem(198)

 ! reactions found in either Trop or Strat but not both
-TYPE(ratb_t), PARAMETER :: ratb_defs_strattrop_aer(1:15)=(/           &
+TYPE(ratb_t), PARAMETER :: ratb_defs_strattrop_aer(1:16)=(/           &
 ratb_t('CS2       ','O(3P)     ','COS       ','SO2       ','CO        ', &
 '         ',3.20e-11,  0.00,    650.00, 0.000, 0.000, 0.000, 0.000) ,  &
 ratb_t('CS2       ','OH        ','COS       ','SO2       ','          ', &
@@ -434,7 +434,9 @@
 ratb_t('Monoterp  ','O3        ','Sec_Org   ','          ','          ', &
 '         ',1.01e-15,  0.00,    732.00, 0.130, 0.000, 0.000, 0.000) ,  &
 ratb_t('Monoterp  ','NO3       ','Sec_Org   ','          ','          ', &
-'         ',1.19e-12,  0.00,   -925.00, 0.130, 0.000, 0.000, 0.000)    &
+'         ',1.19e-12,  0.00,   -925.00, 0.130, 0.000, 0.000, 0.000) ,  &
+ratb_t('ALICE     ','OH        ','BOB       ','Sec_Org   ','          ', &
+'         ',2.70E-11,  0.00,   -390.00, 0.000, 0.000, 0.000, 0.000)    &
   /)

 TYPE(rath_t), ALLOCATABLE :: rath_defs_strattrop_chem(:)
Index: src/atmosphere/UKCA/ukca_setup_chem_mod.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31082)
+++ src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31335)
@@ -262,7 +262,7 @@
     l_ukca_nr_aqchem = .TRUE.
     jpctr            = jpctr + 12
     jpspec           = jpspec + 12
-    jpbk             = jpbk + 15
+    jpbk             = jpbk + 16
     jptk             = jptk + 1
     jppj             = jppj + 4
     jphk             = jphk + 3
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task6.1/task6.1.um.diff** on PUMA.

If you open the **.pk** file in Xconv, you should still see the following fields:

```
 0    : 192   144   36    1     O3 MASS MIXING RATIO
 1    : 192   144   36    1     Molar flux density
 2    : 192   144   85    1     O3 MASS MIXING RATIO
 3    : 192   144   85    1     Field code =  2164
 4    : 192   144   85    1     Field code =  2165
```

Sample output from this task can be found at **`/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task6.1/ai084a.pk19880901`** on ARCHER.

Tutorial 7

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UKCA Chemistry and Aerosol vn10.4 Tutorial 7

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

In this tutorial you will learn how the two UKCA dry deposition schemes are implemented. You will then make changes to allow one of your new tracers to be dry-deposited.

Task 7.1: adding new dry deposition values

TASK 7.1: You should now add in the dry deposition of **ALICE**. This species deposits in a similar way to **CO**. The values for **depvel_defs_strattrop** are:

Surface Type	Summer (day)	Summer (night)	Summer (24h ave)	Winter (day)	Winter (night)	Winter (24h ave)
Water	0.00	0.00	0.00	0.00	0.00	0.00
Forest	0.03	0.03	0.03	0.03	0.03	0.03
Grass	0.03	0.03	0.03	0.03	0.03	0.03
Desert	0.03	0.03	0.03	0.03	0.03	0.03
Ice	0.00	0.00	0.00	0.00	0.00	0.00

i.e. the same as for CO.

Hint [hide]

You will need to make changes for both dry deposition schemes. The changes to **ukca_surfddr.F90** can be made very easily by adding **ALICE** to the **CO** block in the `CASE` statement.

Adding Dry Deposition

UKCA uses two different dry-deposition schemes:

- A simple 2D parameterisation described by Giannakopoulos (1999)[1], Ganzeveld and Lelieveld (1995)[2], and Sander and Crutzen (1996)[3].
- A more detailed interactive parameterisation, based on the Wesely scheme (Wesely, 1989; Sanderson 2007)[4,5]

The default scheme is the interactive scheme, which is chosen by setting `l_ukca_intdd` to **true** in the UKCA panel.

Note: If you are using the interactive scheme and wish to add new values to it, you will also need to add values to the 2D scheme as well, otherwise you will get an error.

During this tutorial you will be tasked with adding the dry deposition of one of your new tracers.

References

1. Giannakopoulos, C., M. P. Chipperfield, K. S. Law, and J. A. Pyle (1999), Validation and intercomparison of wet and dry deposition schemes using 210Pb in a global three-dimensional off-line chemical transport model, J. Geophys. Res., 104(D19), 23761–23784, doi:10.1029/1999JD900392.
2. Ganzeveld, L., and J. Lelieveld (1995), Dry deposition parameterization in a chemistry general circulation model and its influence on the distribution of reactive trace gases, J. Geophys. Res., 100(D10), 20999–21012, doi:10.1029/95JD02266.
3. Sander, R., and P. J. Crutzen (1996), Model study indicating halogen activation and ozone destruction in polluted air masses transported to the sea, J. Geophys. Res., 101(D4), 9121–9138, doi:10.1029/95JD03793.
4. M.L. Wesely, Parameterization of surface resistances to gaseous dry deposition in regional-scale numerical models, Atmospheric Environment (1967), Volume 23, Issue 6, 1989, Pages 1293-1304, ISSN 0004-6981, http://dx.doi.org/10.1016/0004-6981(89)90153-4.
5. Sanderson, M. G., Collins, W. J., Hemming, D. L. and Betts, R. A. (2007), Stomatal conductance changes due to increasing carbon dioxide levels: Projected impact on surface ozone levels. Tellus B, 59: 404–411. doi: 10.1111/j.1600-0889.2007.00277.x

Chemistry Scheme Specification

The default is to use the 2D scheme, although it is advisable to use the interactive scheme. Within the UKCA code, whether a species is dry deposited or not is controlled in the **ukca_chem_scheme.F90** file. In the **chch_defs_scheme** array there are lines like

```
chch_t( 10,'HONO2     ',  1,'TR        ','          ',  1,  1,  0),  & !  10 DD: 7,WD: 4,
chch_t( 11,'H2O2      ',  1,'TR        ','          ',  1,  1,  0),  & !  11 DD: 8,WD: 5,
```

Where the 1 in the 6th column turns on dry deposition of that species (being 0 otherwise). You will need to change the 0 to a **1** for the species that you wish to now dry deposit.

2D Dry Deposition Scheme

The deposition velocities for the 2D scheme are defined in the **depvel_defs_scheme** array, which is held in the **ukca_chem_scheme.F90** module. This is a large array made up of size (6,5) blocks. These blocks mean

Summer (day) velocity over water	Summer (night) velocity over water	Summer (24h ave.) velocity over water	Winter (day) velocity over water	Winter (night) velocity over water	Winter (24h ave.) velocity over water
Summer (day) velocity over forest	Summer (night) velocity over forest	Summer (24h ave.) velocity over forest	Winter (day) velocity over forest	Winter (night) velocity over forest	Winter (24h ave.) velocity over forest
Summer (day) velocity over grass	Summer (night) velocity over grass	Summer (24h ave.) velocity over grass	Winter (day) velocity over grass	Winter (night) velocity over grass	Winter (24h ave.) velocity over grass
Summer (day) velocity over desert	Summer (night) velocity over desert	Summer (24h ave.) velocity over desert	Winter (day) velocity over desert	Winter (night) velocity over desert	Winter (24h ave.) velocity over desert
Summer (day) velocity over ice	Summer (night) velocity over ice	Summer (24h ave.) velocity over ice	Winter (day) velocity over ice	Winter (night) velocity over ice	Winter (24h ave.) velocity over ice

and are in cm/s. The *desert* category is not used, and only the *day* and *night* values are considered in the calculation of the dry-deposition velocities. Examples of these values are

```
!  1  O3 (Ganzeveld & Lelieveld (1995) note 1 (modified to same as Guang)
  0.05,  0.05,  0.05,  0.05,  0.05,  0.05,  & !      1.1
  0.85,  0.30,  0.65,  0.65,  0.25,  0.45,  & !      1.2
  0.65,  0.25,  0.45,  0.65,  0.25,  0.45,  & !      1.3
  0.18,  0.18,  0.18,  0.18,  0.18,  0.18,  & !      1.4
  0.05,  0.05,  0.05,  0.05,  0.05,  0.05,  & !      1.5
!  2  NO (inferred from NO2 - see Giannakopoulos (1998))
  0.00,  0.00,  0.00,  0.00,  0.00,  0.00,  & !      2.1
  0.14,  0.01,  0.07,  0.01,  0.01,  0.01,  & !      2.2
  0.10,  0.01,  0.06,  0.01,  0.01,  0.01,  & !      2.3
  0.01,  0.01,  0.01,  0.01,  0.01,  0.01,  & !      2.4
  0.00,  0.00,  0.00,  0.00,  0.00,  0.00,  & !      2.5
```

Note: When adding new deposition values you should be careful. **UKCA assumes that the order of this array is the same as the order of the species in the chch_defs_scheme array.** If you are adding values for a species in the middle of the list then you will need to make sure that you slot it in to the appropriate place in the existing **depvel_defs_scheme** array (and change the size of this array accordingly). Also note that the dry deposition of the species associated with the aerosol chemistry is held in a separate array which is treated slightly differently. You may find that you need to change the order of the tracers in the `chch_defs` array to accomodate this.

This scheme is controlled in **ukca_ddeprt.F90**. The deposition only occurs in the bottom (i.e. 'surface') layer.

Interactive Dry Deposition Scheme

Adding in new species to the interactive scheme is slightly more involved than for the 2D scheme. This scheme is controlled from the **ukca_ddepctl.F90** routine which is called from *ukca_chemistry_ctl.F90*. The two routines **ukca_aerod.F90** and **ukca_surfddr.F90** contain species specific information, and it is these routines that need to be altered to add in values for a new species. Further details on this scheme can be found in the The UKCA UM documentation paper.

When using this scheme, dry deposition occurs throughout the boundary layer, rather than just in the lowest model (i.e. surface) layer.

Changes to ukca_aerod.F90

This routine calculates the aerodynamic and quasi-laminar surface resistances. The species dependant information that is needed is the diffusion coefficient, **d0** (in units of m^2s^{-1}). By default this is set to -1 if the species is not deposited. If it is deposited, and there are no values for this coefficient in the literature, it is suggested that $d_{0,\text{species}}$ is calculated as

$$d_{0,\text{species}} = d_{0,H_2O}\sqrt{M_{H_2O}/M_{\text{species}}}$$

Where M_{H_2O} is the relative molecular mass of H2O, and M_{species} is the relative molecular mass of the species being deposited, and d_{0,H_2O} is the diffusion coefficient for H2O (2.08E-5 m^2s^{-1}).

You should add in an appropriate value for the new species that you are depositing in the **CASE** statement in this routine. Examples of how this is already done are

```
          CASE ('O3        ','NO2       ','O3S       ','NO3       ')
            d0(j) = 1.4e-5
          CASE ('HONO      ')
            d0(j) = d_h2o * SQRT(m_h2o / m_hono)
```

Note: If you have not yet defined a **M_species** value for your new species, you will need to do this in **ukca_constants.F90**.

Changes to ukca_surfddr.F90

The Wesely scheme considers either 9 different surface types:

1. Broadleaved trees
2. Needleleaf trees
3. C3 Grass
4. C4 Grass
5. Shrub
6. Urban
7. Water
8. Bare Soil
9. Ice

or 13 different surface types:

1. Broadleaved deciduous trees
2. Broadleaved evergreen tropical trees
3. Broadleaved evergreen temperate trees
4. Needleleaf deciduous trees
5. Needleleaf evergreen trees
6. C3 Grass
7. C4 Grass
8. Shrub deciduous
9. Shrub evergreen
10. Urban
11. Water
12. Bare Soil
13. Ice

The examples below are given for 9 surface types, but you will need to make changes for both options.

ukca_surfddr.F90 sets the surface resistance (in sm^{-1}) for each of the species dry-deposited (**rsurf**)). If a species is not deposited onto a particular type of surface (but is deposited onto other types) then its resistance on this type can be set to a very large value (**r_null**). Often many species are assigned the same values. You will need to add in appropriate values for your species into the **CASE** statement within this routine.

Examples of how this is already done are

```
          CASE ('NO2       ','NO3       ')
      rsurf(:,n)=(/225.,225.,400.,400.,600.,1200.,2600.,1200.,       &
        3500. /)
          CASE ('CO        ')
      rsurf(:,n)=(/3700.,7300.,4550.,1960.,4550.0,r_null,r_null,     &
        4550.0,r_null /)  ! Shrub+bare soil set to C3 grass (guess)
```

Increase the value of JPDD

When you added a new chemical reaction you needed to increment a counter which gave the number of reactions, when adding new dry deposition of a species you will need to increase the size of the **JPDD** counter. This is done in the `ukca_setup_chem_mod.F90` module.

Solution to Task 7.1: adding new dry deposition values

You were given the task

- *You should now add in the dry deposition of **ALICE**. This species deposits in a similar way to **CO**. The values for **depvel_defs_strattrop** are:*

Surface Type	Summer (day)	Summer (night)	Summer (24h ave)	Winter (day)	Winter (night)	Winter (24h ave)
Water	0.00	0.00	0.00	0.00	0.00	0.00
Forest	0.03	0.03	0.03	0.03	0.03	0.03
Grass	0.03	0.03	0.03	0.03	0.03	0.03
Desert	0.03	0.03	0.03	0.03	0.03	0.03
Ice	0.00	0.00	0.00	0.00	0.00	0.00

i.e. the same as for CO.

You were given the hint:

- *You will need to make changes for both dry deposition schemes. The changes to **ukca_surfddr.F90** can be made very easily by adding **ALICE** to the **CO** block in the `CASE` statement.*

For a working Rose suite that has completed this task, please see **`u-ai084@26562`**

The specific Rose changes made are (this is just to update the branch revision number):

```
Index: trunk/app/fcm_make_um/rose-app.conf
===================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 26542)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 26562)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task7.1/task7.1.rose.diff** on PUMA.

For a working UM branch that has completed this task, please see **fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@31374**

The specific UM changes made are:

```
Index: src/atmosphere/UKCA/ukca_surfddr.F90
===================================================================
--- src/atmosphere/UKCA/ukca_surfddr.F90        (revision 31335)
+++ src/atmosphere/UKCA/ukca_surfddr.F90        (revision 31374)
@@ -338,7 +338,7 @@
         CASE ('NH3       ')
            rsurf(:,n)=(/137.0,111.1,111.9,131.3,130.4,209.8,196.1,185.8,196.1, &
                         180.7,148.9,213.5,215.1 /)
-        CASE ('CO        ')
+        CASE ('CO        ','ALICE     ')
            rsurf(:,n)=(/3700.0,3700.0,3700.0,7300.0,7300.0,4550.0,1960.0,      &
                         4550.0,4550.0,r_null,r_null,4550.0,r_null /)
            ! Shrub+bare soil set to C3 grass (guess)
@@ -418,7 +418,7 @@
                 500.0, 12500.0 /)
         CASE ('NH3       ')
            rsurf(:,n)=tenpointzero
-        CASE ('CO        ')
+        CASE ('CO        ','ALICE     ')
            rsurf(:,n)=(/3700.0,7300.0,4550.0,1960.0,4550.0,r_null,r_null,   &
                 4550.0,r_null /)  ! Shrub+bare soil set to C3 grass (guess)
         CASE ('CH4       ')
Index: src/atmosphere/UKCA/ukca_chem_strattrop.F90
===================================================================
--- src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31335)
+++ src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31374)
@@ -54,7 +54,7 @@
 INTEGER, PARAMETER, PUBLIC :: nhet_st_tpht   = 2         ! trophet rxns

 ! No of dry deposited species
-INTEGER, PARAMETER, PUBLIC :: ndry_strattrop = 36        ! Stratos chemistry
+INTEGER, PARAMETER, PUBLIC :: ndry_strattrop = 37        ! Stratos chemistry
 INTEGER, PARAMETER, PUBLIC :: ndry_st_aer    = 5         ! Aerosol chemistry

 ! No of wet deposited species
@@ -214,8 +214,8 @@
 chch_t( 74,'O2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  75
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
-!  76
-chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  1),  &
+!  76 DD:37
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  1,  0,  1),  &
 !  77
 chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0)   &
   /)
@@ -371,8 +371,8 @@
 chch_t( 74,'O2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  75
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
-!  76
-chch_t( 76,'ALICE     ',  1,'TR        ','          ',  0,  0,  1),  &
+!  76 DD:37
+chch_t( 76,'ALICE     ',  1,'TR        ','          ',  1,  0,  1),  &
 !  77
 chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0),  &
 !  78
@@ -1020,7 +1020,7 @@

 REAL :: depvel_defs_strattrop01(360)
 REAL :: depvel_defs_strattrop02(360)
-REAL :: depvel_defs_strattrop03(360)
+REAL :: depvel_defs_strattrop03(390)

 INTEGER(KIND=jpim), PARAMETER :: zhook_in  = 0
 INTEGER(KIND=jpim), PARAMETER :: zhook_out = 1
@@ -2580,7 +2580,13 @@
   0.83,  0.04,  0.44,  0.06,  0.05,  0.06,  & !      36.2
   0.63,  0.06,  0.35,  0.08,  0.06,  0.07,  & !      36.3
   0.03,  0.03,  0.03,  0.03,  0.03,  0.03,  & !      36.4
-  0.01,  0.01,  0.01,  0.01,  0.01,  0.01   & !      36.5
+  0.01,  0.01,  0.01,  0.01,  0.01,  0.01,  & !      36.5
+! 37 ALICE as CO (see Giannokopoulos (1998))
```

```
+  0.00,  0.00,  0.00,  0.00,  0.00,  0.00,  & !     37.1
+  0.03,  0.03,  0.03,  0.03,  0.03,  0.03,  & !     37.2
+  0.03,  0.03,  0.03,  0.03,  0.03,  0.03,  & !     37.3
+  0.03,  0.03,  0.03,  0.03,  0.03,  0.03,  & !     37.4
+  0.00,  0.00,  0.00,  0.00,  0.00,  0.00   & !     37.5
   /)


Index: src/atmosphere/UKCA/ukca_aerod.F90
===================================================================
--- src/atmosphere/UKCA/ukca_aerod.F90  (revision 31335)
+++ src/atmosphere/UKCA/ukca_aerod.F90  (revision 31374)
@@ -224,6 +224,8 @@
       d0(j) = d_h2o * SQRT(m_h2o / m_meoh)
     CASE ('Monoterp  ')
       d0(j) = d_h2o * SQRT(m_h2o / m_monoterp)
+    CASE ('ALICE     ')
+      d0(j) = d_h2o * SQRT(m_h2o / m_ALICE)
     END SELECT
   END DO
   !
Index: src/atmosphere/UKCA/ukca_setup_chem_mod.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31335)
+++ src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31374)
@@ -254,7 +254,7 @@
   jptk           = 24
   jppj           = 56
   jphk           = 0
-  jpdd           = 36
+  jpdd           = 37
   jpdw           = 29
   ! If aerosol chemistry on, add additional reactions
   IF (l_ukca_chem_aero) THEN
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task7.1/task7.1.um.diff** on PUMA.

If you open the **.pk** file in Xconv, you should still see the following fields:

```
 0    : 192   144   36    1     O3 MASS MIXING RATIO
 1    : 192   144   36    1     Molar flux density
 2    : 192   144   85    1     O3 MASS MIXING RATIO
 3    : 192   144   85    1     Field code =  2164
 4    : 192   144   85    1     Field code =  2165
```

Sample output from this task can be found at **/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task7.1/ai084a.pk19880901** on ARCHER.

Tutorial 8

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 8

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

In this tutorial you will learn how the wet deposition of chemical species is handelled in UKCA. You will then add-in the wet deposition of one of your new tracers.

Task 8.1: Add wet deposition of a species

Task 8.1: Add in wet deposition for **BOB**, using the following values:

$k(298)$	$-(\Delta H/R)$	$k(298)$ **for the 1st dissociation**	$-(\Delta H/R)$ **for the 1st dissociation**	$k(298)$ **for the 2nd dissociation**	$-(\Delta H/R)$ **for the 2nd dissociation**
$0.21 \times 10^{+06}$	$0.87 \times 10^{+04}$	$0.2 \times 10^{+02}$	0.0	0.0	0.0

Adding Wet Deposition

The formulation used in UKCA is described in Giannakopoulos (1999)[1]. This scheme uses the following formula to calculate the effective Henry's Law coefficient

$$H_{eff} = k\left(298\right)\exp\left(-\frac{\Delta H}{R}\left[\left(\frac{1}{T}\right)-\left(\frac{1}{298}\right)\right]\right)$$

where $k\left(298\right)$ is the rate constant at 298K.

During this tutorial you will be tasked with adding the wet deposition of one of your new tracers.

References

1. Giannakopoulos, C., M. P. Chipperfield, K. S. Law, and J. A. Pyle (1999), Validation and intercomparison of wet and dry deposition schemes using 210Pb in a global three-dimensional off-line chemical transport model, J. Geophys. Res., 104(D19), 23761–23784, doi:10.1029/1999JD900392.

Turning on Wet Deposition for a Species

Chemistry Scheme Specification

Within the UKCA code, whether a species is wet deposited or not is controlled in the **ukca_chem_scheme.F90** file. In the **chch_defs_scheme** array there are lines like

```
chch_t( 10,'HONO2     ',  1,'TR        ','          ',  1,  1,  0),  & !  10 DD: 7,WD: 4,
chch_t( 11,'H2O2      ',  1,'TR        ','          ',  1,  1,  0),  & !  11 DD: 8,WD: 5,
```

Where the 1 in the 7th column turns on wet deposition of that species (being 0 otherwise). You will need to change the 0 to a **1** for the species that you wish to now wet deposit.

Setting Henry's Law values

In the **ukca_chem_scheme.F90** the parameters required to calculate H_{eff} are held in the **henry_defs_scheme** array, and has format

$k(298)$	$-(\Delta H/R)$	$k(298)$ for the 1st dissociation	$-(\Delta H/R)$ for the 1st dissociation	$k(298)$ for the 2nd dissociation	$-(\Delta H/R)$ for the 2nd dissociation

Columns 3 and 4 are used if the species dissociates in the aqueous phase. In this case, H_{eff} is further multiplied by a factor of

$$1 + \frac{k(aq)}{H^{+}}$$

where

$$k(aq) = k\left(298\right) \exp\left(-\frac{\Delta H}{R}\left[\left(\frac{1}{T}\right) - \left(\frac{1}{298}\right)\right]\right)$$

and column 3 contains the values of $k(298)$ and column 4 contains the value of $-\Delta H / R$. Similarly, if the species dissociates a second time then a further factor of $1 + k(aq) / H^{+}$ is applied, where this value of $k(aq)$ is calculated from the values of $k(298)$ and $-\Delta H / R$ in columns 5 and 6.

Note: As with the 2D dry deposition values in **depvel_defs_scheme**, the order of **henry_defs_scheme** also assumes that the values are in the same order as the species (that wet deposit) in the **chch_defs_scheme** array.

Examples for this array are

```
0.2100E+06, 0.8700E+04, 0.2000E+02, 0.0000E+00, 0.0000E+00, 0.0000E+00,&   !    4  HONO2
0.8300E+05, 0.7400E+04, 0.2400E-11,-0.3730E+04, 0.0000E+00, 0.0000E+00,&   !    5  H2O2
```

Increase the value of JPDW

Similar to when adding dry deposition of a species you will need to increase the size of the **JPDW** counter. This is done in the `ukca_setup_chem_mod.F90` module.

Solution to Task 8.1: Add wet deposition of a species

You were given the task

- *Add in wet deposition for **BOB**, using the following values:*

$k(298)$	$-(\Delta H/R)$	$k(298)$ **for the 1st dissociation**	$-(\Delta H/R)$ **for the 1st dissociation**	$k(298)$ **for the 2nd dissociation**	$-(\Delta H/R)$ **for the 2nd dissociation**
$0.21 \times 10^{+06}$	$0.87 \times 10^{+04}$	$0.2 \times 10^{+02}$	0.0	0.0	0.0

For a working Rose suite that has completed this task, please see **`u-ai084@26593`**

The specific Rose changes made are (this is just to update the branch revision number):

```
Index: trunk/app/fcm_make_um/rose-app.conf
===================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 26562)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 26593)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
```

These differences can be found in the file **`/home/ukca/Tutorial/worked_solutions/Task8.1/task8.1.rose.diff`** on PUMA.

For a working UM branch that has completed this task, please see **`fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@31398`**

The specific UM changes made are:

```
Index: src/atmosphere/UKCA/ukca_chem_strattrop.F90
===================================================================
--- src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31374)
+++ src/atmosphere/UKCA/ukca_chem_strattrop.F90 (revision 31398)
@@ -58,8 +58,8 @@
 INTEGER, PARAMETER, PUBLIC :: ndry_st_aer    = 5          ! Aerosol chemistry

 ! No of wet deposited species
-INTEGER, PARAMETER, PUBLIC :: nwet_strattrop = 29         ! Stratos chemistry
-INTEGER, PARAMETER, PUBLIC :: nwet_st_aer    = 34         ! Aerosol chemistry
+INTEGER, PARAMETER, PUBLIC :: nwet_strattrop = 30         ! Stratos chemistry
+INTEGER, PARAMETER, PUBLIC :: nwet_st_aer    = 35         ! Aerosol chemistry


 ! ATA NLA CheST Chemistry v1.2
@@ -216,8 +216,8 @@
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  76 DD:37
 chch_t( 76,'ALICE     ',  1,'TR        ','          ',  1,  0,  1),  &
```

```
-!  77
-chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0)   &
+!  77       WD:30
+chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  1,  0)   &
   /)

 TYPE(chch_t), PUBLIC :: chch_defs_strattrop_aer(1:89)=(/             &
@@ -373,19 +373,19 @@
 chch_t( 75,'N2        ',  1,'CT        ','          ',  0,  0,  0),  &
 !  76 DD:37
 chch_t( 76,'ALICE     ',  1,'TR        ','          ',  1,  0,  1),  &
-!  77
-chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  0,  0),  &
+!  77       WD:31
+chch_t( 77,'BOB       ',  1,'TR        ','          ',  0,  1,  0),  &
 !  78
 chch_t( 78,'DMS       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  79 DD:37,WD:31,EM:10
+!  79 DD:37,WD:32,EM:10
 chch_t( 79,'SO2       ',  1,'TR        ','          ',  1,  1,  1),  &
 !  80
 chch_t( 80,'H2SO4     ',  1,'TR        ','          ',  0,  0,  0),  &
 !  81
 chch_t( 81,'MSA       ',  1,'TR        ','          ',  0,  0,  0),  &
-!  82 DD:38,WD:32
+!  82 DD:38,WD:33
 chch_t( 82,'DMSO      ',  1,'TR        ','          ',  1,  1,  0),  &
-!  83 DD:39,WD:33,EM:11
+!  83 DD:39,WD:34,EM:11
 chch_t( 83,'NH3       ',  1,'TR        ','          ',  1,  1,  1),  &
 !  84
 chch_t( 84,'CS2       ',  1,'TR        ','          ',  0,  0,  0),  &
@@ -397,7 +397,7 @@
 chch_t( 87,'SO3       ',  1,'TR        ','          ',  0,  0,  0),  &
 !  88 DD:40,      EM: 12
 chch_t( 88,'Monoterp  ',  1,'TR        ','          ',  1,  0,  1),  &
-!  89 DD:41,WD:34
+!  89 DD:41,WD:35
 chch_t( 89,'Sec_Org   ',  1,'TR        ','          ',  1,  1,  0)   &
   /)

@@ -914,7 +914,9 @@
 !   28  MeCO2H
  0.4700e+04, 0.6000e+04, 0.1800e-04, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
 !   29  MeOH
- 0.2300e+03, 0.4900e+04, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00 &
+ 0.2300e+03, 0.4900e+04, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
+!   30  BOB
+ 0.2100E+06, 0.8700E+04, 0.2000E+02, 0.0000E+00, 0.0000E+00, 0.0000E+00 &
   /),(/  6, nwet_strattrop/) )


@@ -979,13 +981,15 @@
  0.4700e+04, 0.6000e+04, 0.1800e-04, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
 !   30  MeOH
  0.2300e+03, 0.4900e+04, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
-!   31  SO2
+!   31  BOB
+ 0.2100E+06, 0.8700E+04, 0.2000E+02, 0.0000E+00, 0.0000E+00, 0.0000E+00,&
+!   32  SO2
  0.1230e+01, 0.3020e+04, 0.1230e-01, 0.2010e+04, 0.6000e-07, 0.1120e+04,&
-!   32  DMSO
+!   33  DMSO
  0.5000e+05, 0.6425e+04, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
-!   33  NH3 (H*)
+!   34  NH3 (H*)
  0.1000e+07, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00, 0.0000e+00,&
-!   34  SEC_ORG
+!   35  SEC_ORG
  0.1000e+06, 0.1200e+02, 0.0000e-00, 0.0000e+00, 0.0000e+00, 0.0000e+00 &
  /),(/  6,  nwet_st_aer/) )

Index: src/atmosphere/UKCA/ukca_setup_chem_mod.F90
===================================================================
--- src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31374)
+++ src/atmosphere/UKCA/ukca_setup_chem_mod.F90 (revision 31398)
@@ -255,7 +255,7 @@
    jppj            = 56
    jphk            = 0
    jpdd            = 37
```

```
-  jpdw            = 29
+  jpdw            = 30
   ! If aerosol chemistry on, add additional reactions
   IF (l_ukca_chem_aero) THEN
     l_ukca_achem     =.TRUE.
```

These differences can be found in the file **`/home/ukca/Tutorial/worked_solutions/Task8.1/task8.1.um.diff`** on PUMA.

If you open the **.pk** file in Xconv, you should still see the following fields:

```

 0    : 192   144   36    1     O3 MASS MIXING RATIO
 1    : 192   144   36    1     Molar flux density
 2    : 192   144   85    1     O3 MASS MIXING RATIO
 3    : 192   144   85    1     Field code =  2164
 4    : 192   144   85    1     Field code =  2165
```

Sample output from this task can be found at **`/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task8.1/ai084a.pk19880901`** on ARCHER.

Tutorial 9

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 9

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

In this tutorial you will learn about the UKCA diagnostics package and the different diagnostics that you can output using it. You will also learn how to add new diagnostics from the new reactions and deposition that you have added.

Task 9.1: Output new diagnostics

TASK 9.1: Output diagnostics of the reaction $\mathrm{ALICE} + \mathrm{OH} \longrightarrow \mathrm{BOB} + \mathrm{SEC\_ORG}$ to STASH code **50230**, the dry deposition of **ALICE** to STASH code **50231**, and the wet deposition of **BOB** to **50232**. They should be outputted as a daily mean to the **pk/UPK** stream.

Hint [hide]
Remember to use the correct sampling frequency.

Note:

Adding New UKCA Diagnostics

If you are using one of the chemistry schemes that uses ASAD (e.g. *CheT/TropIsop*, *CheS/Strat*, *CheST/StratTrop*) then you can make use of the ASAD Reaction Flux Diagnostics module (held in **asad_chem_flux_diags.F90**). These allow you to straight-forwardly output new reaction and deposition fluxes.

To output new diagnostics you will first need to define them in the **asad_flux_dat.F90** module, and then create new STASHmaster file specifications for them.

During this tutorial you will be tasked with outputting the reaction and deposition fluxes that you have added in to your branch.

Flux Definitions in asad_flux_dat.F90

Within the **asad_flux_dat.F90** module the diagnostics are defined in blocks with the format

```
    asad_flux_defn('Diagnostic type',STASH code,'Diagnostic specification',Mask,Reaction number,Number of spec
    (/'Species/Reactant 1','Reactant 2'/),
    (/'Product 1','Product 2','Product 3','Product 4'/)),
```

Which have the following meaning:

Diagnostic Type

This is a **three character string** which defines what type of diagnostic is being requested. This can take the values

- **RXN** to output the flux through a reaction (in moles/gridcell/s)
- **DEP** to output the deposition flux of a species (in moles/gridcell/s)
- **NET** to output the net chemical tendency of a species (in moles/gridcell/s)
- **STE** to output the net dynamical tendency of a species (in moles/gridcell/s)
- **MAS** to output the mass of the atmosphere (in kg/gridcell)
- **PSC** to output polar stratospheric cloud diagnostics (1 when the gridcell contains a PSC, 0 otherwise - monthly mean field will be a fraction in range 0 → 1)
- **TPM** to output the tropospheric mask (1 for troposphere, 0 otherwise - monthly mean field will be a fraction in range 0 → 1)
- **OUT** to output a tracer in mmr. Only really useful if the field is masked to give the tropospheric concentration only (see the discussion of the **Mask** option)

STASH Code

This is a **5 digit integer** defining the STASH code that the diagnostic will be outputted to (e.g. 50001). Currently this must be in **section 50**.

Diagnostic Specification

This is a **one character string** which is needed to further define what diagnostic is required. If it isn't needed then it should just be set to **X** or left blank.

- *RXN*
  - **B** to output the flux through a bimolecular reaction
  - **T** to output the flux through a termolecular reaction
  - **H** to output the flux through a heterogeneous reaction
  - **J** to output the flux through a photolysis reaction
- *DEP*
  - **D** to output the dry deposition flux
  - **W** to output the wet deposition flux
- *PSC*
  - **1** to output the fraction of Type 1 PSCs
  - **2** to output the fraction of Type 2 PSCs

Mask

This is a **logical** which defines whether only the tropospheric values of the diagnostic are outputted (**.TRUE.**) or not (**.FALSE.**). It is calculated every timestep.

For the *STE* diagnostic this is required if you wish to output the diagnosed stratosphere-troposphere exchange of a species. For the *OUT* diagnostic this can be used to output only the tropospheric concentration of a tracer. This is also used in the calculation of the of the *TPM* diagnostic.

Reaction number

This is an **integer**, and should only be used in the special case of there being two (or more) reactions with the exactly the same reactants and products, but with different rate coefficients. In this case the first reaction in the list would be given number **1** and the second **2** etc. If this is not needed then it should be set to **0** (which will be usual for most reactions).

Number of Species

This is an **integer**, and should give the total number of species, so this will be **1** for diagnostics such as *DEP*, *STE*, *NET* etc., which only consider a single species, and the **total number of reactants and products** for diagnostics *RXN* and *RTE*.

Species

This is a **10-character string** giving the exact name of the species that the diagnostic should be considered for (including capitalisation). This is only used for the *DEP*, *NET*, *STE*, and *OUT*. For the *RXN* and *RTE* diagnostics the full list of reactants and products should be given (see below). For the *MAS*, *PSC*, and *TPM* diagnostics this isn't needed and could either be set to **XXX** or left blank. If it is needed the other reactant/product slots should be left blank.

Reactants and Products

These are **10-character strings**, and should be as the reaction is defined in the **ukca_chem_scheme.F90** modules.

Addition of Diagnostics

If you define more than one diagnostic to be output to the same STASH code, then the diagnostic routines will sum these diagnostics together. This can be useful (e.g., if you wanted to output the sum of all NO+RO2 reactions to one STASH item), but can be problematic if you accidentally output two fields to the same STASH code, as this will give strange results!

Changes to `asad_flux_dat.F90`

After you have defined your new diagnostics at the top of this module, you will need to make sure that they have been added correctly to the **asad_chemical_fluxes** array, which is defined in the **ASAD_LOAD_DEFAULT_FLUXES** subroutine held in the **asad_flux_dat.F90**.

Changes to `asad_chem_flux_diags.F90`

You will need to edit `asad_chem_flux_diags.F90` if you want to output a new type of diagnostic. This can be quite involved, but you can look at existing routines to see how things are done. Also, you will probably need to increment the **`nmax_chemdiags`** counter, which is essentially the maximum *STASH item number* in section 50 that this routine will write to.

STASHmaster file

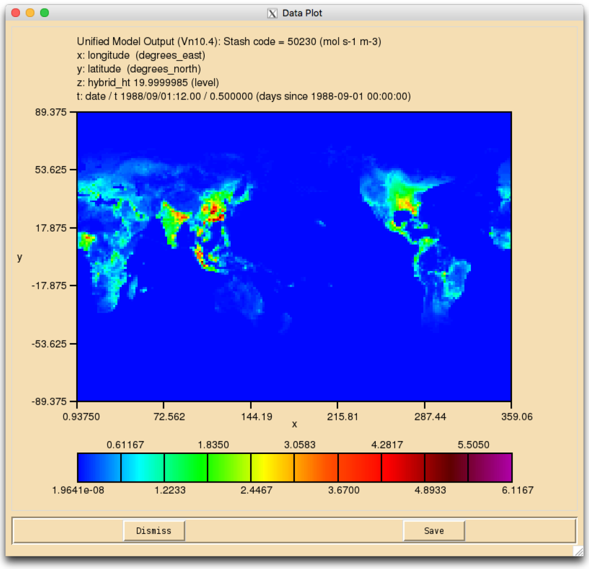
While the diagnostics are defined in **asad_flux_dat.F90** they are turned on by requesting the item through STASH. To do this you will need to edit the STASHmaster_A file in your branch.

Most UKCA diagnostics are 3D, although some, such as emissions (which are outputted in a different way), are 2D. You should take care with the STASH settings in STASHmaster_A between these types, as there some differences that will need to be considered.

Rose Changes

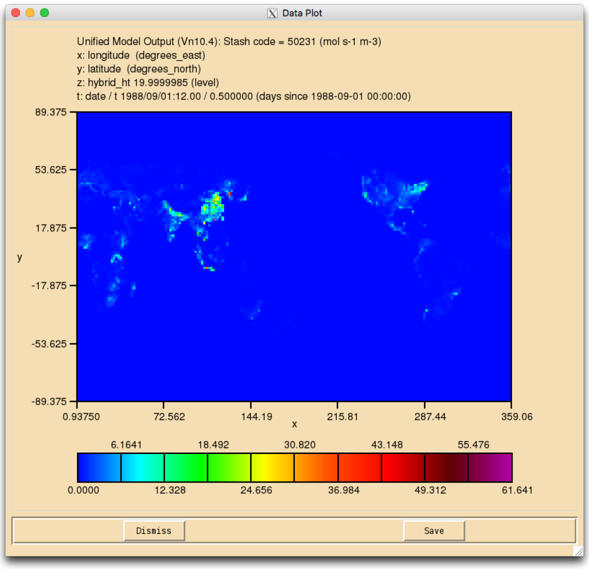
After you have made your STASmaster_A file changes, you will need to add these diagnostics into STASH, as per Tutorial 3. Remember to run the TidyStashTransform macro. If you included this STASHmaster_A file using *@HEAD*, you won't need to make any further changes to Rose, but you will need to make sure that you have committed your UM branch prior to running. Because the file is taken from *`fcm:um.xm_br`* you will need to make sure that the revision has synced to the PUMA mirror (i.e. by waiting a few minutes).

Solution to Task 9.1: Output new diagnostics



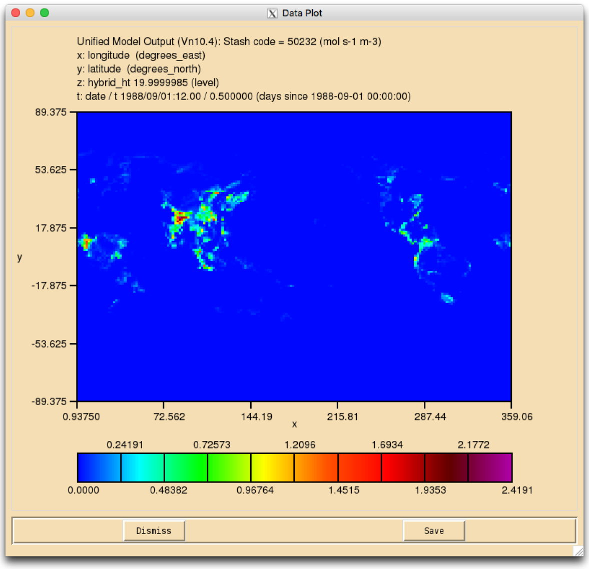
Unified Model Output (Vn10.4): Stash code = 50230 (mol s-1 m-3)
x: longitude (degrees_east)
y: latitude (degrees_north)
z: hybrid_ht 19.9999985 (level)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)

ALICE + OH → BOB + Sec_Org (s50i230) reaction flux (mol/s) at the surface (20m)



Unified Model Output (Vn10.4): Stash code = 50231 (mol s-1 m-3)
x: longitude (degrees_east)
y: latitude (degrees_north)
z: hybrid_ht 19.9999985 (level)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)

ALICE dry deposition flux (s50i231) (mol/s) at the surface (20m)



Unified Model Output (Vn10.4): Stash code = 50232 (mol s-1 m-3)
x: longitude (degrees_east)
y: latitude (degrees_north)
z: hybrid_ht 19.9999985 (level)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)

BOB wet deposition flux (s50i232) (mol/s) at the surface (20m)

You were given the task

- Output diagnostics of the reaction $\mathrm{ALICE} + \mathrm{OH} \longrightarrow \mathrm{BOB} + \mathrm{SEC\_ORG}$ to STASH code **50230**, the dry deposition of **ALICE** to STASH code **50231**, and the wet deposition of **BOB** to **50232**. They should be outputted as a daily mean to the **pk/UPK** stream.

You were given the hint:

- *Remember to use the correct sampling frequency.*

For a working Rose suite that has completed this task, please see **`u-ai084@26618`**

The specific Rose changes made are:

```
Index: trunk/app/um/rose-app.conf
===================================================================
--- trunk/app/um/rose-app.conf  (revision 26593)
+++ trunk/app/um/rose-app.conf  (revision 26618)
@@ -7534,6 +7534,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'
```

```
+[namelist:streq(8d9d5406)]
+dom_name='DALLTH'
+isec=50
+item=230
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(8db529bf)]
 dom_name='DIAG'
 isec=5
@@ -7838,6 +7846,14 @@
 tim_name='TALLTS'
 use_name='UPUKCA'

+[namelist:streq(9b488d41)]
+dom_name='DALLTH'
+isec=50
+item=231
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(9c7680fe)]
 dom_name='DSOIL'
 isec=8
@@ -9366,6 +9382,14 @@
 tim_name='TMPMN15'
 use_name='UPMEAN'

+[namelist:streq(e03d06b7)]
+dom_name='DALLTH'
+isec=50
+item=232
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(e063ae3a)]
 dom_name='DALLRH'
 isec=0
Index: trunk/app/fcm_make_um/rose-app.conf
===================================================================
--- trunk/app/fcm_make_um/rose-app.conf (revision 26593)
+++ trunk/app/fcm_make_um/rose-app.conf (revision 26618)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tro
```

These differences can be found in the file **/home/ukca/Tutorial/worked_solutions/Task9.1/task9.1.rose.diff** on PUMA.

For a working UM branch that has completed this task, please see **fcm:um.x_br/dev/lukeabraham/vn10.4_UKCA_Tutorial_Solns@31422**

The specific UM changes made are:

```

Index: src/atmosphere/UKCA/asad_flux_dat.F90
===================================================================
--- src/atmosphere/UKCA/asad_flux_dat.F90       (revision 31398)
+++ src/atmosphere/UKCA/asad_flux_dat.F90       (revision 31422)
@@ -97,7 +97,7 @@
 CHARACTER(LEN=10) :: blank0 = '          '   ! Defines null product

 ! Number of chemical fluxes defined below
-INTEGER, PARAMETER :: n_chemical_fluxes = 232
+INTEGER, PARAMETER :: n_chemical_fluxes = 235

 TYPE(asad_flux_defn), ALLOCATABLE, SAVE :: asad_chemical_fluxes(:)

@@ -1022,6 +1022,19 @@

 TYPE(asad_flux_defn), PUBLIC :: asad_aerosol_chem(16)

+TYPE(asad_flux_defn), PARAMETER, PUBLIC ::                        &
+                                    ukca_tutorial_fluxes(3) = (/ &
+asad_flux_defn('RXN',50230,'B',.FALSE.,0,4,                       &
+(/'ALICE     ','OH        '/),                                    &

+(/'BOB       ','Sec_Org   ','          ','          '/)),        &
+asad_flux_defn('DEP',50231,'D',.FALSE.,0,1,                      &
+(/'ALICE     ','          '/),                                   &
+(/'          ','          ','          ','          '/)),        &
+asad_flux_defn('DEP',50232,'W',.FALSE.,0,1,                      &
+(/'BOB       ','          '/),                                   &
+(/'          ','          ','          ','          '/))         &
+/)
+
 PUBLIC :: asad_load_default_fluxes

   CHARACTER(LEN=*), PARAMETER, PRIVATE :: ModuleName='ASAD_FLUX_DAT'
@@ -1096,7 +1109,8 @@
    asad_strat_oh_loss,          & ! 26 181
    asad_strat_o3_budget,        & ! 20 201
    asad_strat_o3_misc,          & ! 15 216
-   asad_aerosol_chem            & ! 16 232
+   asad_aerosol_chem,           & ! 16 232
+   ukca_tutorial_fluxes         & ! 3  235
    /)

 IF (printstatus >= PrStatus_Normal) THEN
Index: src/atmosphere/UKCA/asad_chem_flux_diags.F90
===================================================================
--- src/atmosphere/UKCA/asad_chem_flux_diags.F90        (revision 31398)
+++ src/atmosphere/UKCA/asad_chem_flux_diags.F90        (revision 31422)
@@ -158,7 +158,7 @@
 TYPE(stashsumdiag), DIMENSION(:), ALLOCATABLE, SAVE ::            &
                                              stash_handling

-INTEGER, PARAMETER :: nmax_chemdiags = 205      ! For CJ
+INTEGER, PARAMETER :: nmax_chemdiags = 232      ! For CJ
 INTEGER, SAVE :: n_chemdiags

 REAL, ALLOCATABLE, DIMENSION(:,:,:) :: temp_chemdiag
Index: rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf
===================================================================
--- rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf (revision 31398)
+++ rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster-meta.conf (revision 31422)
@@ -17800,6 +17800,21 @@
     =
     =Available if chemistry and photolysis are turned ON in UKCA

+[stashmaster:code(50230)]
+description=RXN FLUX: ALICE+OH->BOB+Sec_Org
+help=Flux through ALICE+OH->BOB+Sec_Org reaction
+    =moles/s
+
+[stashmaster:code(50231)]
+description=DRY DEP FLUX: ALICE
+help=Dry Deposition flux of ALICE (3D)
+    =moles/s
+
+[stashmaster:code(50232)]
+description=WET DEP FLUX: BOB
+help=Wet Deposition flux of BOB (3D)
+    =moles/s
+
 [stashmaster:code(51001)]
 description=O3 MASS MIXING RATIO ON PRESS LEVS
 help=Ozone Mass Mixing Ratio in kg/kg(Air)
@@ -20228,6 +20243,21 @@
     =This is the sum of all species contributing to NOy in a
     =given chemistry scheme

+[stashmaster:code(52230)]
+description=RXN FLUX: ALICE+OH->BOB+Sec_Org PLEV
+help=Flux through ALICE+OH->BOB+Sec_Org reaction on pressure levels
+    =moles/s
+
+[stashmaster:code(52231)]
+description=DRY DEP FLUX: ALICE PRESSURE LEVELS
+help=Dry Deposition flux of ALICE (3D) on pressure levels
+    =moles/s
+
+[stashmaster:code(52232)]
+description=WET DEP FLUX: BOB PRESSURE LEVELS
+help=Wet Deposition flux of BOB (3D) on pressure levels
+    =moles/s
+
 [stashmaster:code(53181)]
 description=Temperature Inc: Idealised  (K/step)
 help=Temperature increment from the idealised section in Kelvin per model
Index: rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A
===================================================================
--- rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A (revision 31398)
+++ rose-meta/um-atmos/HEAD/etc/stash/STASHmaster/STASHmaster_A (revision 31422)
@@ -21441,6 +21441,24 @@
 4|    1 |    0 | -17  -17  -17  -17  -21  16   -17  -99  -99  -99 |
 5|    0 | 3829 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
 #
+1|    1 |   50 |  230 |RXN FLUX: ALICE+OH->BOB+Sec_Org     |
+2|    0 |    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 | 1871 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   50 |  231 |DRY DEP FLUX: ALICE                 |
+2|    0 |    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 | 1871 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   50 |  232 |WET DEP FLUX: BOB                   |
+2|    0 |    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 | 1871 |    0 |   65 |    0 |    0 |    0 |    0 |    0 |
+#
 #==============================================================================
 # Section 50 Item 999 reserved.
 #==============================================================================
@@ -23615,6 +23633,24 @@
 4|    1 |    0 | -17  -17  -17  -17  -21  16   -17  -99  -99  -99 |
 5|    0 | 3829 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
 #
+1|    1 |   52 |  230 |RXN FLUX: ALICE+OH->BOB+Sec_Org PLEV|
+2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
+3| 000000000000000000000000000000 | 00000000000000000001 |    3 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 1871 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   52 |  231 |DRY DEP FLUX: ALICE PRESSURE LEVELS |
+2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
+3| 000000000000000000000000000000 | 00000000000000000001 |    3 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 1871 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
+#
+1|    1 |   52 |  232 |WET DEP FLUX: BOB PRESSURE LEVELS   |
+2|    0 |    0 |    1 |    1 |    3 |    1 |    2 |    0 |    0 |    0 |    1 |
+3| 000000000000000000000000000000 | 00000000000000000001 |    3 |
+4|    1 |    0 | -99  -99  -99  -99  -99  -99  -99  -99  -99  -99 |
+5|    0 | 1871 |    0 |    8 |    0 |    0 |    0 |    0 |    0 |
+#
 #==============================================================================
 # Section 52 Item 999 reserved.
 #==============================================================================
```

These differences can be found in the file **`/home/ukca/Tutorial/worked_solutions/Task9.1/task9.1.um.diff`** on PUMA.

If you open the **.pk** file in Xconv, you should now see the following fields:

```
0    : 192   144   36    1     O3 MASS MIXING RATIO
1    : 192   144   36    1     Molar flux density
2    : 192   144   85    1     O3 MASS MIXING RATIO
3    : 192   144   85    1     Field code =  2164
4    : 192   144   85    1     Field code =  2165
5    : 192   144   85    1     Molar flux density
6    : 192   144   85    1     Molar flux density
7    : 192   144   85    1     Molar flux density
```

Sample output from this task can be found at **`/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task9.1/ai084a.pk19880901`** on ARCHER.

Tutorial 10

Written by Luke Abraham 2016

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UKCA Chemistry and Aerosol vn10.4 Tutorial 10

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

In this tutorial you will learn about *aerosol optical depth* (AOD) and how to request AOD diagnostics from UKCA. We will explain how aerosol optical properties are calculated by the RADAER module, based on the size-resolved aerosol simulated by the GLOMAP aerosol microphysics scheme.

Note: The GLOMAP aerosol tutorials require you to use `u-ai071` and work from that for these tasks.

Task 10.1: What is aerosol optical depth and how do I request AOD diagnostics in UKCA?

Aerosol particles affect the Earth's radiative balance by scattering and absorbing solar radiation and, where they are large enough, can also act similarly to a greenhouse gas by absorbing outgoing terrestrial long-wave radiation.

The aerosol optical depth (AOD), sometimes referred to as aerosol optical thickness (AOT), is often used in atmospheric science as a measure of how strongly the aerosol particles within an air mass extinguish radiation (either by scattering it or absorbing it). The AOD can be thought of as a indicator of the strength of aerosol-radiation interactions at a particular wavelength.

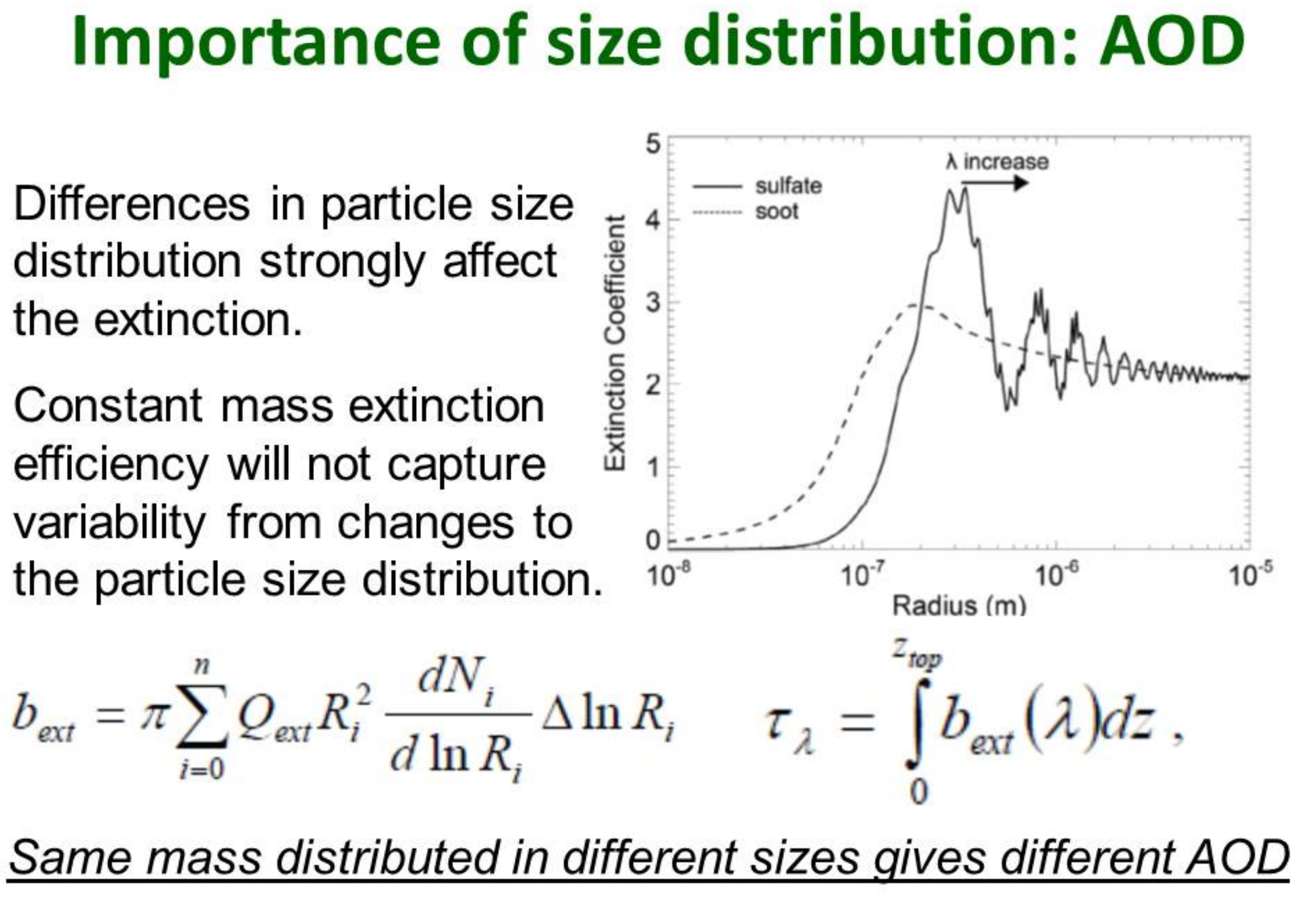
The AOD is defined as the vertical integral of the monochromatic (single-wavelength) extinction (the sum of scattering plus absorption) through the atmospheric column. It is common also to refer to an absorption AOD which represents the integral of just the single-wavelength absorption.

The Unified Model (UM) radiation scheme divides the shortwave (SW) and longwave (LW) spectra into wavebands. To enable UKCA simulated gases or aerosols to interact with the UM radiation scheme, their optical properties need to be integrated across each of these wavebands. For aerosols, the radiation scheme requires the specific scattering and absorption coefficients, which describe the strength of aerosol scattering and absorption processes per unit aerosol mass (in $m^2\ kg^{-1}$), and the asymmetry parameter, which describes in a simplified way the angular dependence of the scattering (dimensionless). The specific scattering and absorption coefficients, and the asymmetry parameter, are hereafter referred to as the *aerosol optical properties*.

Task 10.2: Understand the principles behind GLOMAP and how aerosol optical properties are derived via RADAER

Mie theory describes the scattering and absorption of light by spherical particles. Essentially, the scattering/absorption efficiency can be parameterized in terms of two parameters: the (complex) refractive index of the particle and the Mie parameter, which describes the particle size dependence in relation to the wavelength of light under consideration.

The Figure in the slide below shows the dependence on particle size of the extinction efficiency for mid-visible (550nm, green) light for two different types of particle (refractive index).



Importance of size distribution: AOD

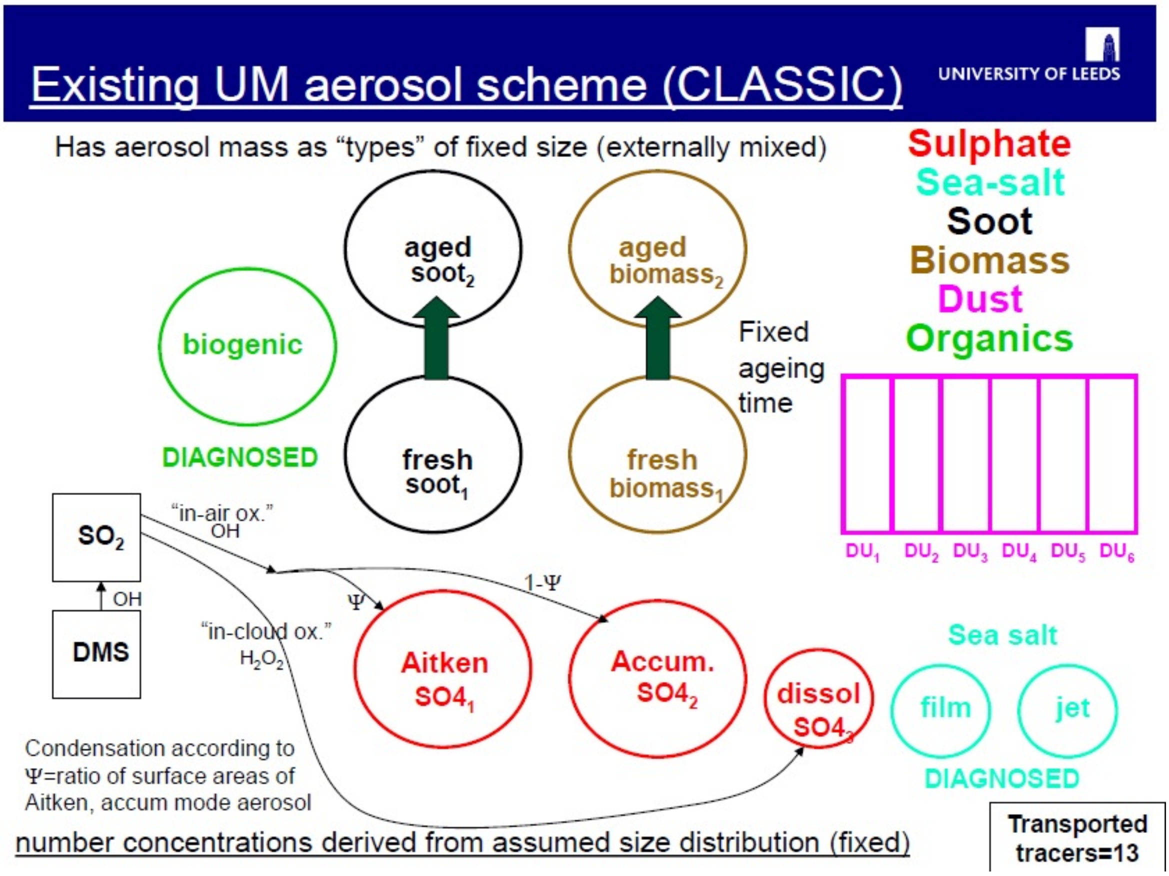
Differences in particle size distribution strongly affect the extinction.

Constant mass extinction efficiency will not capture variability from changes to the particle size distribution.

$$b_{ext} = \pi \sum_{i=0}^{n} Q_{ext} R_i^2 \frac{dN_i}{d\ln R_i} \Delta \ln R_i \qquad \tau_\lambda = \int_0^{z_{top}} b_{ext}(\lambda)\, dz \ ,$$

Same mass distributed in different sizes gives different AOD

The aerosol scheme used for UK climate model simulations in CMIP5 was a simplified mass-based scheme Coupled Large-scale Aerosol Simulator for Studies In Climate (CLASSIC, e.g. Bellouin et al., 2007). Although CLASSIC is simpler than the microphysical GLOMAP scheme included in UKCA, it does have a comprehensive representation of the main aerosol sources, tracking up to eight tropospheric aerosol species: ammonium sulphate, mineral dust, fossil fuel black carbon (soot), fossil fuel organic carbon, biomass burning aerosols, sea-salt, secondary organic (also called biogenic), and ammonium nitrate aerosols. The first 5 of these are treated interactively in terms of their mass, but prescribe globally and temporally uniform values for their size distribution and refractive index. Some variation in aerosol properties was resolved by having fresh and aged sub-types for some of these types, which then allow size and refractive index to vary from values near-source (fresh) to remote (aged).



Existing UM aerosol scheme (CLASSIC)

Has aerosol mass as "types" of fixed size (externally mixed)

Condensation according to Ψ=ratio of surface areas of Aitken, accum mode aerosol

number concentrations derived from assumed size distribution (fixed)

Transported tracers=13

With this simplified approach, optical properties for each aerosol type are derived based on Mie calculations using the uniform size distribution and refractive index for each type with water uptake based on a fixed hygroscopic growth factor. For all three properties the constants used are based on average values observed in air masses dominated by the particular type.

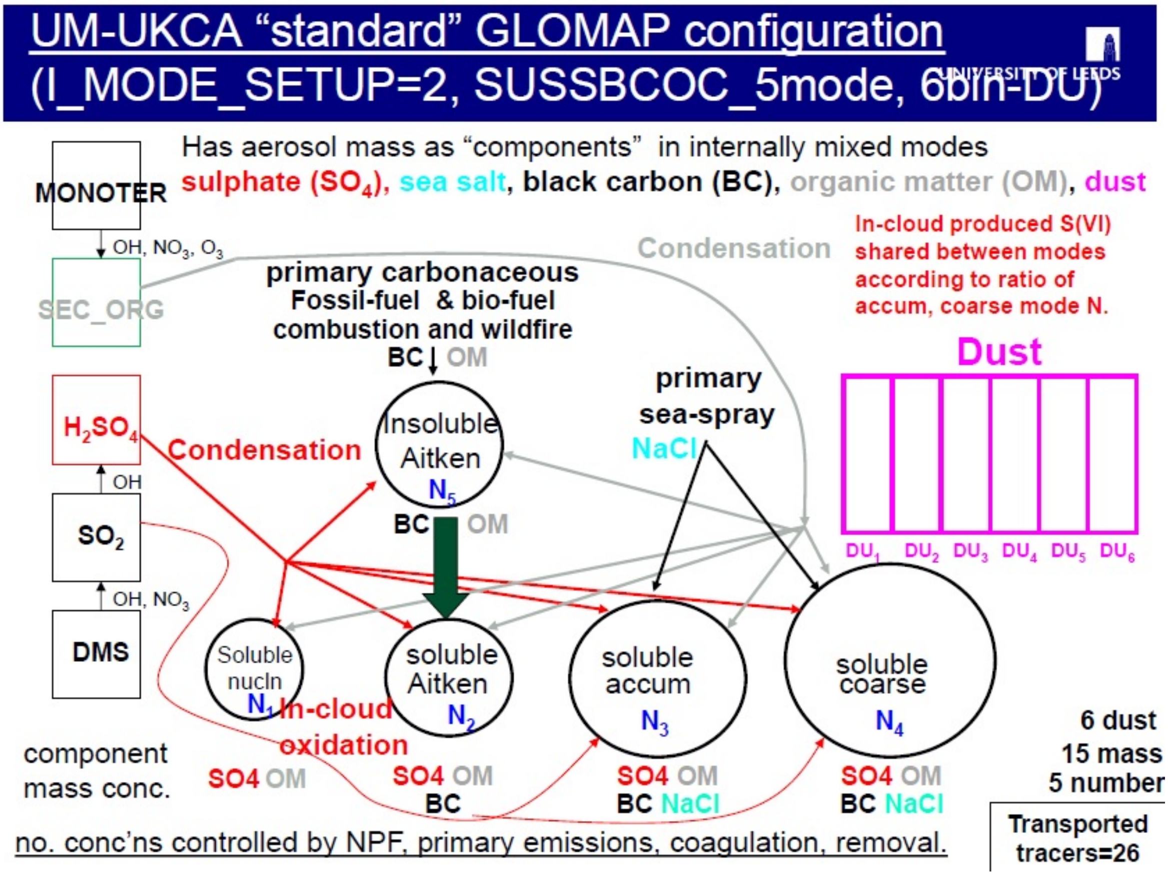
The GLOMAP-mode aerosol scheme in UKCA differs in that it simulates the variation of size-resolved aerosol properties, as they evolve due to microphysical processes such as new particle formation, coagulation, condensation (gas-to-particle-transfer) and cloud processing.

Whereas CLASSIC simulated only the mass of several aerosol types, the transported tracers in GLOMAP are particle number and mass in different size classes spanning the particle size range from 3nm up to around 20 microns dry diameter.

Processes such as condensation and aqueous sulphate production grow particles to larger sizes by increasing the mass in a size class while conserving particle number.

As was as microphysical processes, GLOMAP also includes size-resolved representations of primary emissions (e.g. of sea-salt, dust and carbonaceous particles), and also has size-resolved removal processes including particle dry deposition, sedimentation, nucleation scavenging (rainout) and impaction scavenging (washout).

GLOMAP therefore simulates the evolution of particle number and composition across the size spectrum over several different chemical constituents or components (e.g. sea-salt, sulphate, black carbon) as determined by the aerosol processes included.



UM-UKCA "standard" GLOMAP configuration (I_MODE_SETUP=2, SUSSBCOC_5mode, 6bin-DU)

Has aerosol mass as "components" in internally mixed modes sulphate (SO_4), sea salt, black carbon (BC), organic matter (OM), dust

6 dust
15 mass
5 number

no. conc'ns controlled by NPF, primary emissions, coagulation, removal.

Transported tracers=26

The original version of GLOMAP (known as GLOMAP-bin) uses a two-moment sectional aerosol dynamics approach, with typically 20 bins spanning the size spectrum, but when tracking several aerosol types, becomes too expensive for running multi-decadal integrations as required in a climate model. For UKCA, a new computationally cheaper version of GLOMAP was developed (GLOMAP-mode), which has the same process representations, but using log-normal modes as its size classes. Each size mode in GLOMAP-mode covers one of four size ranges (nucleation, Aitken, accumulation, coarse), and additionally distinguishing between soluble and insoluble modes.

GLOMAP has been developed to follow a flexible multi-component approach, with the same code able to be run with different levels of composition/size sophistication with FORTRAN-90 modules providing alternative aerosol *mode set-up* arrays. The GLOMAP-mode aerosol scheme in UKCA not only simulates the dry aerosol mass, but also the mass of water attached to the aerosol, and the aerosol number concentrations.

The calculation of aerosol optical properties from GLOMAP is carried out by the RADAER module included in UKCA.

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

- The mean radius of each size class (mode) varies in time and space as determined by transport and aerosol processes.
- There is a refractive index for each size class (mode) which varies according to its internally-mixed composition.
- The aerosol water taken up into each soluble mode varies interactively, consistently with particle composition.

RADAER relies on pre-computed look-up tables of monochromatic optical properties, covering all realistic combinations of modal radii and refractive indices. At runtime, remaining tasks are:

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

As well as providing the waveband-averaged scattering, extinction and asymmetry parameters from GLOMAP, RADAER also diagnoses monochromatic Aerosol Optical Depth (AOD) for each of the GLOMAP modes.

Task 10.3: Output daily-mean Aerosol Optical Depths from your UKCA model run

In this task you will update your copy of the UKCA tutorial suite (`u-ai071`) adding extra STASH requests to output daily-mean AODs from GLOMAP.

UM-UKCA diagnoses the AOD from each of the GLOMAP modes as a separate STASH item.

All of the GLOMAP AOD diagnostics are contained with STASH section 2 (long-wave radiation) in item numbers close to those used for the AOD diagnostics from CLASSIC.

Section 2 items 300-305 contain the AOD for the Aitken-soluble, accumulation-soluble, coarse-soluble, Aitken-insoluble, accumulation-insoluble and coarse-insoluble modes respectively.

The dimensions for each of these STASH items is 2D global in longitude and latitude but there is also a third dimension containing 6 pseudo levels for the 6 monochromatic AODs stored by the model (at 0.38, 0.44, 0.55, 0.67, 0.87, 1.02 micron wavelengths).

Note that there is no nucleation mode AOD as those particles are too small to significantly scatter or absorb radiation at these wavelengths.

There are separate "stratospheric AOD" diagnostics in section 2 items 251 to 256 which can also be requested to store the AOD in levels above the tropopause.

Note there are also absorption AOD in these 6 modes can usually be requested via STASH section 2 items 240 to 245, in the job here these are not available in the UKCA tutorial suite.

To output AODs from GLOMAP, you need to add in some extra STASH requests for the section 2 items 300 to 305.

To output as a daily-mean select the usage profile "UPK" to output to the .pk files and the time profile "TDAYM" for daily-means. For AOD STASH requests, you need to select the domain profile DIAGAOT to output over the longitude, latitude and 6 wavelength pseudo-levels.

In the next task (Task 11), you will change the GLOMAP aerosol setup to have two different OM components in each size mode, to allow to track two different types of particulate OM. In anticipation of that task, as well as the AOD for each mode, we'll also request the mass mixing ratio of OM in each mode.

Section 34 items 106, 110, 116, 121 and 126 contain the OM mmr's in the Aitken-soluble, accumulation-soluble, coarse-soluble, Aitken-insoluble and nucleation-soluble modes respectively.

When requesting the OM mmr's, use the DALLTH domain profile, as those variables are on the full 3D model grid.

After doing that you will have an equivalent version of the UKCA tutorial job with a number of additional *daily-mean fields* requested.

Since you specified the UPK usage profile in the job, these fields will be output to the so-called *.pk files.*

These can be found in your /work/n02/n02/ directory on ARCHER. You should have a file like **jobid**a.pk19880901 for the daily-mean fields for the 1 day that the job was set to run for.

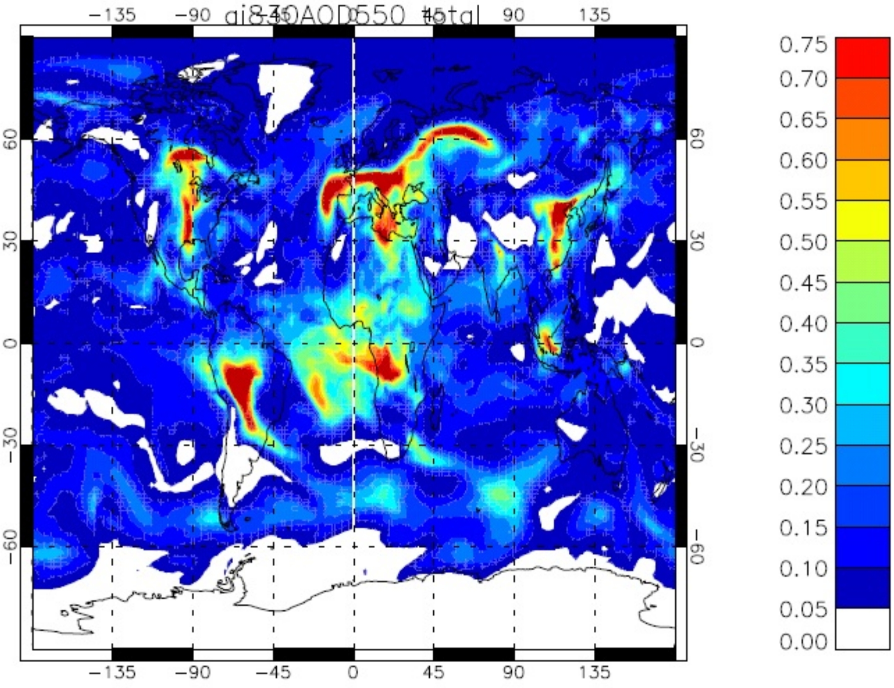
In the first instance you should use xconv to open the file although you can use convsh or other tools to extract required fields from the .pk file and then manipulate them in IDL or python.

As an example I have put below a jpeg showing a global map produced in IDL of the daily-mean AOD at 550nm (total over all modes) for 1st September 1988 from the UKCA tutorial suite (worked solution `u-ai830`).

In preparation for the next task, you should also re-run the job adding also daily-mean STASH requests for the following mass mixing ratios (mmr's) for the Organic Matter (OM) in each mode (34106, 34110, 34116, 34121 and 34126).

Once you have re-run the job with these extra fields available in the .pk file, you can use the cdo operator *cdo add* to sum up each of the OM mmrs to give a total OM mmr in a separate netCDF file.

You should now `cd` into your `$HOME/roses/[SUITE-ID]` directory and `fcm commit` your changes.



Worked Solution

A worked solution to **Task 10.3** is job `u-ai830`.

Your .pk file will contain the following fields:

```
0     : 192    144    6      1      Unspecified
1     : 192    144    6      1      Unspecified
2     : 192    144    6      1      Unspecified
```

```
3    : 192   144   6     1     Unspecified
4    : 192   144   6     1     Unspecified
5    : 192   144   6     1     Unspecified
6    : 192   144   6     1     Unspecified
7    : 192   144   6     1     Unspecified
8    : 192   144   6     1     Unspecified
9    : 192   144   6     1     Unspecified
10   : 192   144   6     1     Unspecified
11   : 192   144   6     1     Unspecified
12   : 192   144   85    1     AITKEN MODE (SOLUBLE) OC MMR
13   : 192   144   85    1     ACCUMULATION MODE (SOL) OC MMR
14   : 192   144   85    1     COARSE MODE (SOLUBLE) OC MMR
15   : 192   144   85    1     AITKEN MODE (INSOLUBLE) OC MMR
16   : 192   144   85    1     NUCLEATION MODE (SOLUBLE) OC  MMR
```

You can use **cdo** as so to add the 5 separate netCDF files containing the OC mass-mixing ratios. To do this you must first

```
module load cdo
```

to give you access to the command. You can extract the required fields from the .pk file using Xconv or convsh. An example convsh script is below:

```
#! /usr/bin/env convsh

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4

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# Written by N. Luke Abraham 2017-01-06 <nla27@cam.ac.uk>

# you should change the input file name here
readfile 0 ai922a.pk19880901

# You may need to change the field numbers (first column in Xconv or when using list_fields)
# You should also change the prepended suite-id
# These should match these names:
#  AITKEN MODE (SOLUBLE) OC MMR
writefile netcdf ai922_m01s34i106.nc 12
#  ACCUMULATION MODE (SOL) OC MMR
writefile netcdf ai922_m01s34i110.nc 13
#  COARSE MODE (SOLUBLE) OC MMR
writefile netcdf ai922_m01s34i116.nc 14
#  AITKEN MODE (INSOLUBLE) OC MMR
writefile netcdf ai922_m01s34i121.nc 15
#  NUCLEATION MODE (SOLUBLE) OC  MMR
writefile netcdf ai922_m01s34i126.nc 16
```

These can then be combined using the following cdo command:

```
cdo add ai922_m01s34i106.nc -add ai922_m01s34i110.nc -add ai922_m01s34i116.nc -add ai922_m01s34i121.nc ai922_m01s34i126.nc ai922_OCmmr_cdo.nc
```

When opening the output file (`ai922_OCmmr_cdo.nc` in the example above) the variable name is taken from the first file in the list.

It is also possible to use Iris to extract and combine these fields - an example script showing how to do this is below:

```
#!/usr/bin/env python

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4

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# version.

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# You find a copy of the GNU Lesser General Public License at <http://www.gnu.org/licenses/>.

# Written by N. Luke Abraham 2017-01-06 <nla27@cam.ac.uk>

# preamble
import iris

# load all OC components
oc=iris.load('./ai922a.pk19880901',
        [iris.AttributeConstraint(STASH='m01s34i106'),
        iris.AttributeConstraint(STASH='m01s34i110'),
        iris.AttributeConstraint(STASH='m01s34i116'),
        iris.AttributeConstraint(STASH='m01s34i121'),
        iris.AttributeConstraint(STASH='m01s34i126')])

# make cube to store total OC
ocsum=oc[0].copy()

# add-up components
ocsum.data=oc[0].data+oc[1].data+oc[2].data+oc[3].data+oc[4].data

# rename
ocsum.rename('mass_fraction_of_total_particulate_organic_matter_in_air')

# remove unlimited dimension when writing to netCDF
iris.FUTURE.netcdf_no_unlimited=True

```

```
# output to netCDF
iris.save(ocsum,'ai922_OCmmr_iris.nc',netcdf_format='NETCDF3_CLASSIC')
```

It is also possible to use Iris to calculate the 0.55 micron AOD - an example script to do this is below:

```
#!/usr/bin/env python

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4

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# Written by N. Luke Abraham 2017-01-06 <nla27@cam.ac.uk>

# preamble
import iris

# load all AOD components at 0.55 micron
aod=iris.load('./ai922a.pk19880901',
        [iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i300'),
        iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i301'),
        iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i302'),
        iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i303'),
        iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i304'),
        iris.Constraint(pseudo_level=3) & iris.AttributeConstraint(STASH='m01s02i305')])

# make cube to store total AOD
aodsum=aod[0].copy()

# add-up components
aodsum.data=aod[0].data+aod[1].data+aod[2].data+aod[3].data+aod[4].data+aod[5].data

# rename
aodsum.rename('atmosphere_optical_thickness_due_to_aerosol')

# remove unlimited dimension when writing to netCDF
iris.FUTURE.netcdf_no_unlimited=True

# output to netCDF
iris.save(aodsum,'ai922_AOD_iris.nc',netcdf_format='NETCDF3_CLASSIC')
```

Example output can be found on ARCHER in the directory

```
/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task10.3
```

The Rose-specific changes can be found in the file

```
/home/ukca/Tutorial/worked_solutions/Task10.3/task10.3.rose.diff
```

on PUMA

```
Index: app/um/rose-app.conf
===================================================================
--- app/um/rose-app.conf        (revision 28511)
+++ app/um/rose-app.conf        (revision 28536)
@@ -4862,6 +4862,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(1cdb7a57)]
+dom_name='DALLTH'
+isec=34
+item=106
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(1cedac0b)]
 dom_name='DIAG'
 isec=3
@@ -4886,6 +4894,14 @@
 tim_name='TDAYM'
 use_name='UPD'

+[namelist:streq(1d51d9e9)]
+dom_name='DALLTH'
+isec=34
+item=116
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(1d882b73)]
 dom_name='DIAG'
 isec=1
@@ -4934,6 +4950,14 @@
 tim_name='T90DAY'
 use_name='UPI'

+[namelist:streq(1fa7073a)]
+dom_name='DALLTH'
+isec=34
+item=126
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(1fbc22ae)]
 dom_name='DP17'
 isec=30
@@ -6454,6 +6478,14 @@
 tim_name='TMPMN18'
 use_name='UPMEAN'

+[namelist:streq(5e6e0742)]
+dom_name='DALLTH'
+isec=34
+item=110
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(5f297582)]
 dom_name='DIAG'
 isec=30
@@ -6606,6 +6638,14 @@
 tim_name='TRADDM'
 use_name='UPMEAN'

+[namelist:streq(67a9602e)]
+dom_name='DIAGAOT'
+isec=2
+item=254
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(67e9519f)]
 dom_name='DALLTH'
 isec=1
@@ -6686,6 +6726,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(6b285660)]
+dom_name='DIAGAOT'
+isec=2
+item=255
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(6b37b902)]
 dom_name='DIAG'
 isec=1
@@ -6782,6 +6830,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(6ebee303)]
+dom_name='DIAGAOT'
+isec=2
+item=252
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(6ec24c21)]
 dom_name='DTROP'
 isec=5
@@ -6902,6 +6958,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(74c20937)]
+dom_name='DIAGAOT'
+isec=2
+item=256
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(75413c65)]
 dom_name='DTROP'
 isec=5
@@ -7550,6 +7614,14 @@
 tim_name='TALLTS'
 use_name='UPUKCA'

+[namelist:streq(8f865257)]
+dom_name='DALLTH'
+isec=34
+item=121
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(8fc8c95a)]
 dom_name='DNOGWTH'
 isec=6
@@ -7830,6 +7902,14 @@
 tim_name='T6HDMPM'
 use_name='UPMEAN'

+[namelist:streq(9f3b2872)]
+dom_name='DIAGAOT'
+isec=2
+item=253
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(9f60f084)]
 dom_name='DIAG'
 isec=1
@@ -8262,6 +8342,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(b45df417)]
+dom_name='DIAGAOT'
+isec=2
+item=300
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(b4656f70)]
 dom_name='DIAG'
 isec=4
@@ -8438,6 +8526,14 @@
 tim_name='TDAYM'
 use_name='UPD'

+[namelist:streq(bb6af665)]
+dom_name='DIAGAOT'
+isec=2
+item=251
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(bccca6bc)]
 dom_name='DIAG'
 isec=5
@@ -8678,6 +8774,14 @@
 tim_name='TMPMN00'
 use_name='UPMEAN'

+[namelist:streq(c49b9649)]
+dom_name='DIAGAOT'
+isec=2
+item=303
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(c5a142ea)]
 dom_name='DIAG'
 isec=3
@@ -9390,6 +9494,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(e3f9fc46)]
+dom_name='DIAGAOT'
+isec=2
+item=305
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(e40c8701)]
 dom_name='DIAG'
 isec=5
@@ -9494,6 +9606,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(e924a4a3)]
+dom_name='DIAGAOT'
+isec=2
+item=304
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(e92db8ee)]
 dom_name='DALLTH'
 isec=50
@@ -9646,6 +9766,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(f1347f13)]
+dom_name='DIAGAOT'
+isec=2
+item=302
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(f14e5386)]
 dom_name='DIAG'
 isec=3
@@ -9790,6 +9918,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(f5e063cb)]
+dom_name='DIAGAOT'
+isec=2
+item=301
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(f5e615d1)]
 dom_name='DIAG'
 isec=5
Index: rose-suite.conf
===================================================================
--- rose-suite.conf     (revision 28511)
+++ rose-suite.conf     (revision 28536)
@@ -1,7 +1,7 @@
 [jinja2:suite.rc]
 !!ACCOUNT_USR='foundation'
 ANCIL_OPT_KEYS=
-ARCHER_GROUP='n02-chem'
+ARCHER_GROUP='n02-training'
 ARCHER_QUEUE='short'
 !!ARCH_LOG=true
 !!ARCH_WALL=true
@@ -21,7 +21,7 @@
 !!HOST_XC40='xc'
 HOUSEKEEP=true
 !!HPC_QUEUE='normal'
-HPC_USER='luke'
+HPC_USER='ncastr01'
```

```
HYPTHR_ATM=1
HYPTHR_RCF=1
IOS_NPROC=0
```

Tutorial 11

Written by Graham Mann 2016

UKCA Chemistry and Aerosol vn10.4 Tutorial 11

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

Before you start this tutorial, you should `cd` into your `$HOME/roses/[SUITE-ID]` directory and `fcm commit` your changes.

You should complete this Tutorial using a copy of your working (& committed suite) from Tutorial 10, so please copy this suite now and work from your new copy.

In this tutorial you will learn about the GLOMAP-mode aerosol module and how it tracks different aerosol types within several size classes. You will understand the standard configuration used in the UKCA jobs so far whereby the mass mixing ratios of sulphate, sea-salt, black carbon and organic matter in each mode are transported via separate tracers. GLOMAP-mode is an aerosol microphysics scheme and therefore, as well as transporting the mass of several components in the modes, the scheme also transports the number concentrations of particles in each mode.

Task 10 already introduced the basic concepts behind the GLOMAP-mode aerosol microphysics scheme and how it differs from the mass-based CLASSIC scheme which preceded UKCA.

Initially developed in the TOMCAT CTM environment (see Manktelow et al., 2007; Mann et al., 2010; Mann et al., 2012), the GLOMAP code then became the aerosol module for the UKCA sub-model of the UM (see Bellouin et al., 2013; Kipling et al., 2013; West et al., 2014; Mann et al., 2014; Dhomse et al., 2014; Turnock et al., 2015; Turnock et al., 2016; Zanchettin et al., 2016).

GLOMAP is now also implemented into the ECMWF Integrated Forecasting System as part of the "Composition IFS" module (C-IFS) where it will be used in combination with data assimilation of satellite Aerosol Optical Depth to provide forecasts and re-analyses of atmospheric composition and boundary conditions for regional air quality models. The shift from the current operational aerosol scheme in C-IFS over to GLOMAP-mode is scheduled to take place during 2018.

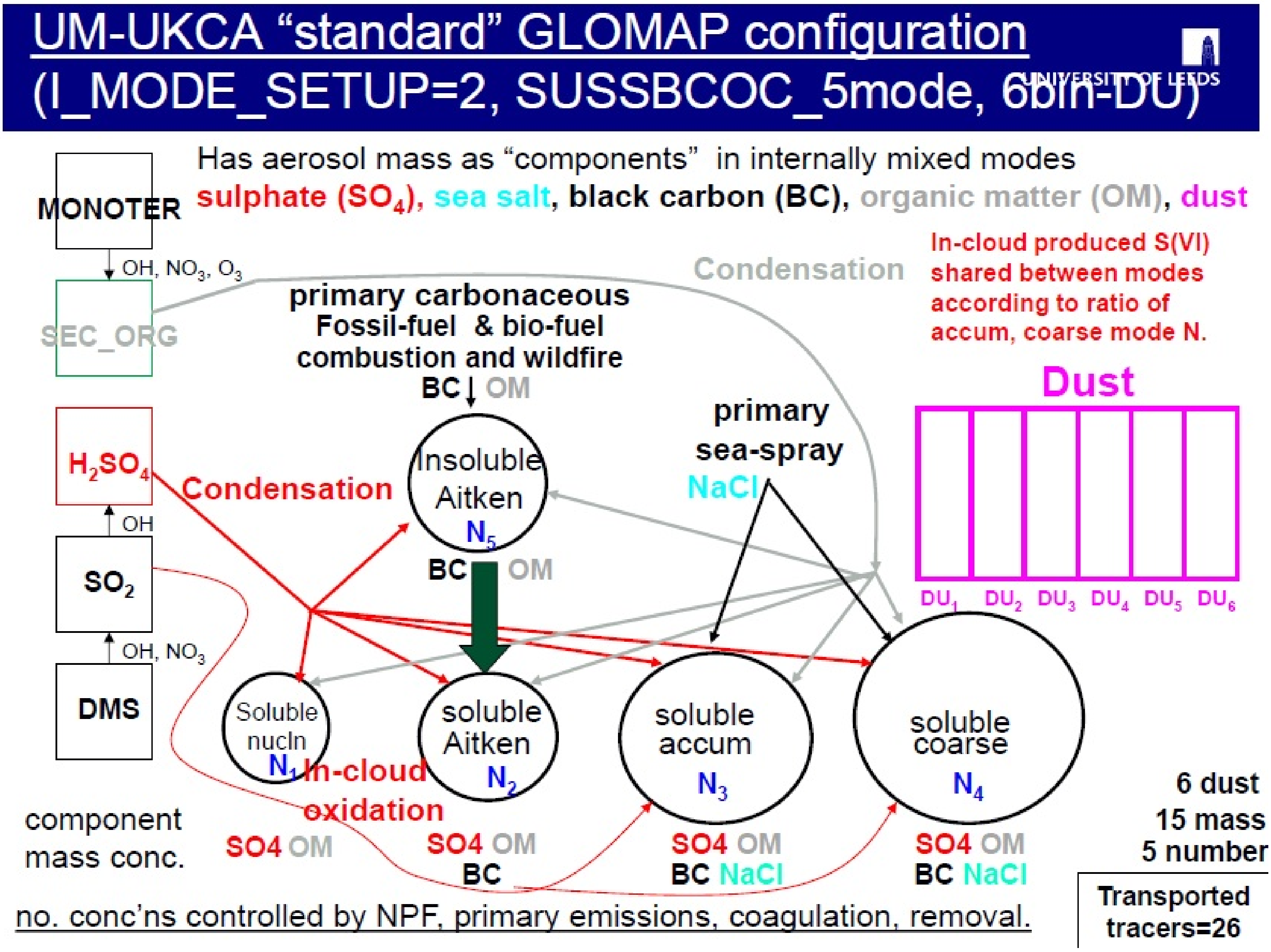
The GLOMAP-mode code allows several alternative "aerosol configurations" to be run using the same set of FORTRAN subroutines.

In section 12 of the UKCA UMDP, Table 18 shows the standard configuration for GLOMAP in both of these other 2 host model frameworks (TOMCAT and C-IFS-GLOMAP).

In this 7-mode configuration (known as setup 8), GLOMAP runs with all 7 modes activated, with 2 being pure dust modes and the other 5 containing mixtures of different aerosol components (sulphate, black carbon, organic matter, sea-salt and dust).

With this GLOMAP setup 8, the model runs has 7 number mixing ratios (one for each mode) and has a total of 19 component mass mixing ratios over all the different types.

As mentioned in task 10 however, when GLOMAP is run within UM-UKCA, dust is usually handled by the existing 6-bin UM scheme, and GLOMAP is configured to use the "5-mode configuration" (known as setup 2) covering only 4 of the above 5 components (sulphate, black carbon, organic matter and sea-salt).



UM-UKCA "standard" GLOMAP configuration (I_MODE_SETUP=2, SUSSBCOC_5mode, 6bin-DU)

Has aerosol mass as "components" in internally mixed modes sulphate (SO_4), sea salt, black carbon (BC), organic matter (OM), dust

In-cloud produced S(VI) shared between modes according to ratio of accum, coarse mode N.

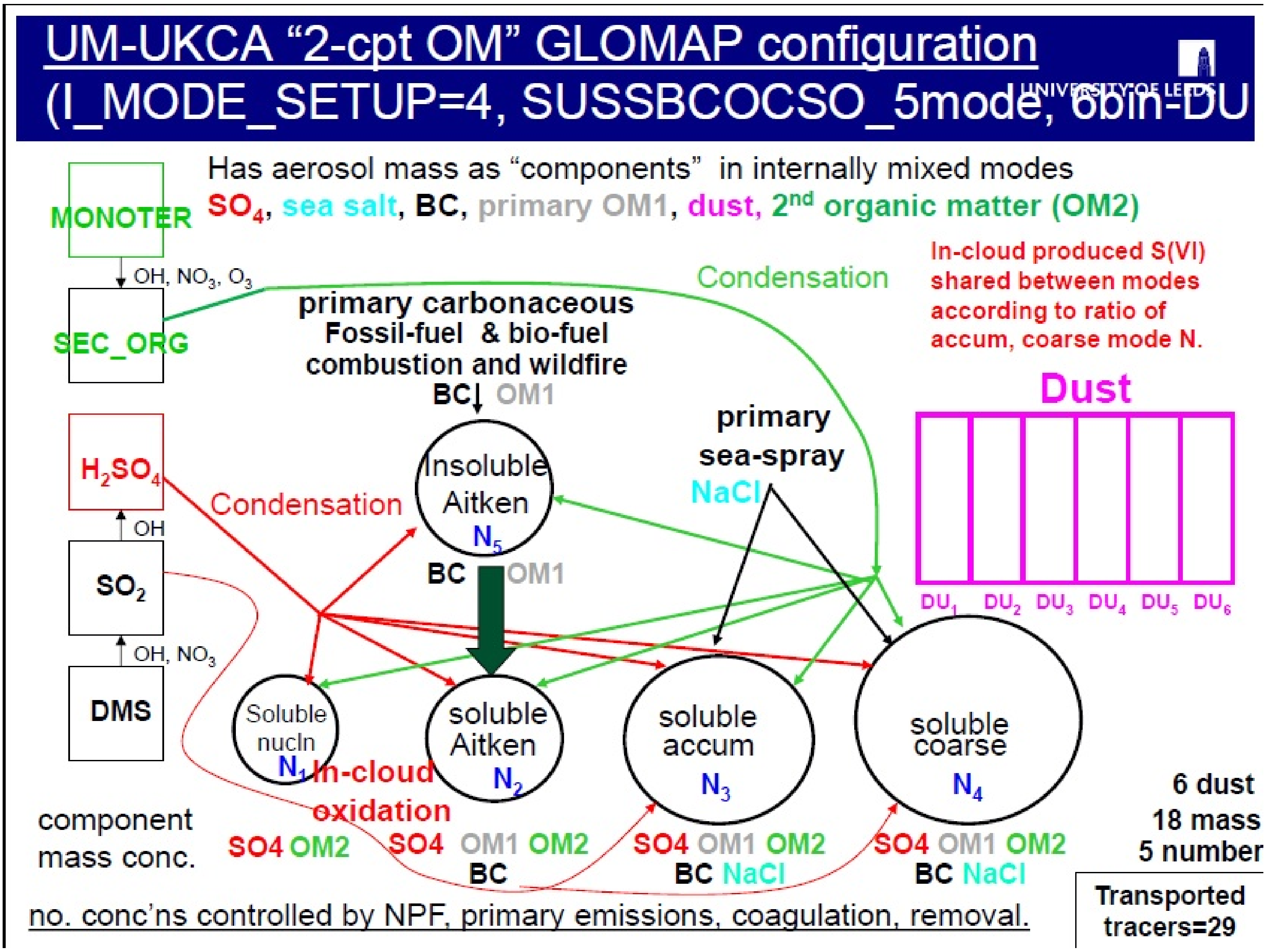
6 dust 15 mass 5 number

Transported tracers=26

no. conc'ns controlled by NPF, primary emissions, coagulation, removal.

The scheme can also be further reduced to cover just the sulphate and sea-salt components in 4 modes (known as setup 1), which was the initial configuration used for interactive stratospheric aerosol simulations (e.g. Dhomse et al., 2014).

The GLOMAP scheme has been run in the TOMCAT CTM in a range of configurations, including one specifically designed to track two separate components for organic matter (OM), with the I_MODE_SETUP=4 configuration designed to have one component track the primary OM in each mode and a separate OM component to track secondary organic matter in each mode.



UM-UKCA "2-cpt OM" GLOMAP configuration
(I_MODE_SETUP=4, SUSSBCOCSO_5mode, 6bin-DU

Has aerosol mass as "components" in internally mixed modes
SO_4, sea salt, BC, primary OM1, dust, 2nd organic matter (OM2)

In-cloud produced S(VI) shared between modes according to ratio of accum, coarse mode N.

component mass conc.

no. conc'ns controlled by NPF, primary emissions, coagulation, removal.

6 dust
18 mass
5 number

Transported tracers=29

Section 12.2 of the UMDP has a more detailed explaination of these configurations with Table 19 showing how these 4 different *GLOMAP-mode setups* map onto the model tracers.

In this task you will take a copy of the standard UKCA job (which uses GLOMAP-mode setup 2, MS2) and change it to use GLOMAP-mode setup 4 (MS4) to track two separate organic matter (OM) components rather than the usual 1. With the 2-component OC configuration, the model tracks primary (emitted) organic carbon in the usual OM component and secondary organic matter (formed following oxidation in the atmosphere) separately in a 2nd OM component.

Task 11.1: Understand how the GLOMAP aerosol module tracks aerosol species and modes

TASK 11.1: Read section 14 (page 51) of the vn10.4 UKCA Unified Model Documentation Paper (UMDP084) (https://code.metoffice.gov.uk/doc/um/vn10.4/umdp.html) and refer to Tables 28, 29 on pages 53.

Task 11.2: Run a copy of the standard UKCA job which tracks two OM components in the GLOMAP modes

Take a copy of the suite you generated from Task 10 with the GLOMAP AOD diagnostics added. This was your copy of the standard ARCHER v10.4 UKCA tutorial suite (u-ai071). The task is to change the aerosol settings from the standard GLOMAP aerosol configuration (setup 2) to instead use the 2-component OM configuration (setup 4).

To run the 2-component GLOMAP configuration, you will need to add in an additional branch to the suite (which supports that) and also make change to the Rose GUI metadata for the suite, so that an extra option for I_MODE_SETUP=4 is made available within the "GLOMAP configuration" selection-button.

First, add in the extra branch. Go to the fcm_make_um app (4th from the top) and then click on "env" then "Sources" which then shows you the 4 branches that are already used in the UKCA tutorial job. These 4 branches are to enable additional settings over and above what was present in the UM trunk code at v10.4.

To add in the extra branch click the plus sign and then paste the following into the new entry that appears after you click the plus:

```
branches/dev/grahammann/vn10.4_support_GLOMAPsetup4_for_2cptOM@32315
```

This is telling to the model that, when the source-code is built, it needs to pick up the code-changes from revision 32315 of the branch I put together to enable UM-UKCA to correctly align with the code that is present in GLOMAP for setup 4 (and adds a few bits that were missing in the v10.4 trunk).

Next we'll need to change the GLOMAP setup. In the Rose GUI, you need to open the UM app (click on the right-hand-pointing triangle at the bottom next to "um") and then similarly click on "namelist" then "UM Science settings" and finally you can then select "Section 34: UKCA" to view which options have been selected in this particular UKCA tutorial job.

There are a long set of different switches which specify how this particular UM-UKCA is configured. Scrolling down (a fair way down) you will see the GLOMAP aerosol setting options listed as *Set aerosol species and modes.* This basically specifies the value for *i_mode_setup*, which controls the GLOMAP aerosol configuration (as explained above). In the tutorial job you can see I_MODE_SETUP has been set to 2. That corresponds to the "standard GLOMAP setup" explained and illustrated above (sulphate, sea-salt, black carbon and one organic carbon component in 5 modes).

You see also that there are alternative options there that can change the aerosol setup to 1 (sulphate and sea-salt in 4 modes), 6 (dust-only in 2 modes) and 8 (sulphate, sea-salt, BC, POM and dust in all 7 modes).

In our case, we actually want a different set-up though to any of these standard 4 options -- to activate to use the 2-component organic matter configuration. Of course one needs to know that that configuration is actually available in the code, and although this is explained in the UMDP, it turns out that, at this version, the I_MODE_SETUP=1, 6 and 8 configurations are not supported, and we recommend you do not select those options without corresponding closely with the GLOMAP development team at Leeds.

In order to do this requires to point the Rose GUI to an updated version of the metadata that provides the information for the different panels in the GUI. At the moment, the metadata used in the job tells the UM that the only options available are I_MODE_SETUP=1, 2, 6 and 8. But with the changes implemented in the branch above, it is then possible to also run the model with I_MODE_SETUP=4 (which is the GLOMAP configuration that we want to run with).

The metadata for the *UM app* within the Rose GUI panel is specified in the first panel selection in the GUI. Instead of clicking on the right-hand-pointing triangle, click on the word *um* and then you should see a panel with only one entry that says "meta" with the text set as:

```
/home/grenville/meta/ga7_vn10.4
```

This is pointing to a rose-meta.conf file that specifies the metadata for the UM app. It is off Grenville Lister's directory because there were things that were decided were required to be added (chosen according to some priorities or requirements) to the functionality of that UM app at that particular time.

In preparation for this task I have updated those Rose selections to additionally allow the user to select the option 4 as well as those 1, 2, 6 and 8.

For this task we need to change the text set in that box to instead be set as:

```
/home/gmann/meta/ga7_vn10.4_MS4updated
```

and then click apply. I have updated the rose-meta.conf metadata file to add the required to enable the extra I_MODE_SETUP=4 to be selected in the GUI.

To get an idea of what is different about the rose-meta.conf file, that then allows the user to choose that option, you could use a graphical difference engine like "tkdiff" or "xxdiff" to compare the rose-meta.conf in those two directories.

```
tkdiff /home/grenville/meta/ga7_vn10.4/rose-meta.conf /home/gmann/meta/ga7_vn10.4_MS4updated/rose-meta.conf
```

By doing this, you see that the functionality that was added in the file off Grenville Lister's directory was to retain the information in the existing rose-meta.conf, but additional add a new switch to allow the user to scale up or down how much NOx is emitted from lightning sources.

In the rose-meta.conf for the *MS4updated* version of this, the code does the same to retain the existing settings set in the rose-meta.conf in the branch, and adds in the new lightnight NOx scaling, but then also provides a replacement for the existing I_MODE_SETUP metadata to allow I_MODE_SETUP to take 5 alternative values (1, 2, 4, 6 and 8) instead of the existing 4.

Once you have changed the text to point to that new meta data file, the button-selection in the UKCA panel changes to having those 5 options rather than the previous 4. Now that the new I_MODE_SETUP=4 option is visible in the Rose GUI, proceed to select that I_MODE_SETUP=4 rather than the previous (default) setting of I_MODE_SETUP=2.

The FORTRAN in the model source-code is (with the updated branch added above) able then to act on the new I_MODE_SETUP specied in the Rose GUI, and activate the required extra OM2 tracers (section 34 items 128, 129, 130 and 131) and also does several other things to enable the code to then have the condensation of SEC_ORG go into the SO component mmrs instead of the OM component mmrs as was the case for I_MODE_SETUP=2.

Note that at previous versions of the UM (v7.3, v8.4), to add the extra tracers for the new I_MODE_SETUP required a UMUI hand-edit to edit the file *SIZES*, setting the values of the array *TC_UKCA* [which specifies which of the UKCA tracers are switched on (=1) or off (=0)]. By contrast, at v10.4, the control for which tracers should be on or off is done based on what is set in the STASHmaster_A file. There is some code within one of the UKCA routines (tstmask_ukca_mod.F90) that interprets one of the fields set in the STASHmaster_A.

If you have not encountered the so-called "STASHmaster_A" file before, it is basically the file that specifies the properties of all the different prognostic and diagnostic variables that are set to be used by the UM.

The STASHmaster_A file is not easy to understand, and it will not be possible to explain many aspects of what it does -- but suffice it to say that it contains a sequence of 5-line segments for each prognostic or diagnostic variable, with several different fields within it, which conveniently specify a range of information about that particular prognostic/diagnostic's properties (that are interpeted within the FORTRAN code of the model when it runs).

The UKCA prognostic variables can be found in section 34 in items 1-150. All the aerosol optical properties diagnostics (e.g. as explained in Task 10), such as the AOD for each mode, can be found in section 2. (Although strictly speaking this section 2 is principally to store long-wave radiation diagnostics, the aerosol optical properties are also stored here for historical reasons.)

The reason I explain this is that we will refer to the STASHmaster_A file to see the way the main UKCA tracers are specified as on or off for the different I_MODE_SETUPs. And you need to be able to appreciate the context of the GLOMAP tracers that have been activated, in relation to the other variables set for the other parts of the model

We will see that this automatic configuring the tracers is actually done from within one of the fields in the STASHmaster *option code* entry. The user-prognostic fields required by other parts of the model (e.g. partial volumes for RADAER, CDNC diags for ACTIVATE, aerosol surface area for heterogeneous chemistry) are also able to be conveniently controlled by a similar approach making the extra fields for the different I_MODE_SETUPs available automatically based on what is set in the STASHmaster_A.

Which of the GLOMAP tracers are switched ON for different GLOMAP configurations (values of I_MODE_SETUP) is controlled by a 30-character string on the 3rd line of the STASHmaster_A entry for that variable. This 30-character string is known as an *option code.* By switched ON I mean it is then set to be a transported tracer and thereby made available during run-time.

If you are familiar with FORTRAN it is worth taking a look at the STASHmaster and also referring to the code where this is done. And for this reason, I recommend at this point that you do an "FCM checkout" (to your local space on PUMA) of the v10.4 branch that was added above.

If you haven't already, you should create an "FCM" directory off your home directory on PUMA. This is where you will store *checkouts* of branches that you have created (or want to refer to). After cd'ing into that directory, run the following command to "check-out" the code in the branch to a "user working copy" in your ~/FCM directory. The command is:

```
fcm checkout fcm:um.x_br/dev/grahammann/vn10.4_support_GLOMAPsetup4_for_2cptOM
```

That checks-out the whole contents of that branch to your ~/FCM/ directory and may take a few minutes to complete (although sometimes it's much quicker).

To look at the STASHmaster_A file, cd into that branch "vn10.4_support_GLOMAPsetup4_for_2cptOM" and then into the following directory within the branch:

```
cd rose-meta/um-atmos/HEAD/etc/stash/STASHmaster
```

you will see the STASHmaster_A file.

It's a big file but if you go to line 14028 (e.g. use capital-G in vi) you see section 34 item 101 and on the 3rd line you see the 30-character string of zeros and ones for *nucleation mode (soluble) number* is set as "100000000000000000000010001011".

The way the model has been coded is to pick up the values of 1 or 0 near the end of this "option code" and use these to specify which tracers are switched on. In short, the nth character from the right-hand side specifies whether the tracer is switched on for I_MODE_SETUP=n.

You see that the 29th and 30th characters are set to "1" which means that the tracer is included for I_MODE_SETUP=1 and I_MODE_SETUP=2. You'll recall that the only other values for I_MODE_SETUP that are allowed to be selected at this model version (in the unchanged base job that is) are I_MODE_SETUP=6 (2mode dust-only) and I_MODE_SETUP=8 (the "full" setup with all 7 modes active). And you see that the 6th-from-the-right is a zero which means that the nucleation mode number tracer is not included in that I_MODE_SETUP=6 configuration (dust-only). But you see that the 8th-from-the-right is set to "1" which means that the tracer is included for I_MODE_SETUP=8 (the "full" set-up with all 7 modes active).

For this task, my branch has additionally activated an extra GLOMAP set-up -- and see that I have edited the STASHmaster to put a 1 also in the 4th character from the end so that that particular tracer is selected to be *switched on* for the I_MODE_SETUP=4 option which is now available.

That's different from the default specification for this tracer (in the UM trunk at v10.4) which specifies the option code as zero for this column 26:

```
100000000000000000000010000011
```

You see in the STASHmaster_A file there are the two sets of organic matter tracers, the first one being called "OC" and the second one called "SO". At some points in the model the tracers are given short-hand names of *Ait_SOL_OC* (item 106), *Acc_SOL_OC* (110), *Cor_SOL_OC* (116), *Ait_INS_OC* (121) and *Nuc_SOL_OC* (126) while the second OM tracers have short names *Nuc_SOL_SO* (128), *Ait_SOL_SO* (129), *Acc_SOL_SO* (130) and *Cor_SOL_SO* (131). But the STASHmaster_A file has their full names -- and you can see that whereas the "OC" tracers are included for both I_MODE_SETUP=2 and I_MODE_SETUP=4, the "SO" tracers are only included for I_MODE_SETUP=4.

The extra tracers for the OM2 mass mixing ratios in each are stored in STASH items 128, 129, 130 and 131 in section 34. You see that these are set to 1 for the SO components in each of the soluble modes and the nucleation soluble OC mmr is no longer required as it has been replaced with SO mmr for that particular mode.

When we changed the Rose GUI to allow the user to select I_MODE_SETUP=4, we did this by pointing the Rose GUI to an updated rose-meta.conf file in a separate directory that enabled the I_MODE_SETUP=4 option. It was this one:

```
/home/gmann/meta/ga7_vn10.4_MS4updated/rose-meta.conf
```

The reason I refresh the memory about this is to further explain that, in a sub-directory of that same "ga7_vn10.4_MS4updated" main directory, the "MS4-updated" version of the STASHmaster_A file that I included in the branch is also identically present there (with the I_MODE_SETUP=4 option enabled). This copy of the "MS4-updated" STASHmaster_A file can be found at:

```
/home/gmann/meta/ga7_vn10.4_MS4updated/etc/stash/STASHmaster
```

Due to a quirk in this preliminary realisation of the Rose software (which is still in its infancy really for use with the UM), when one makes a change to the STASHmaster_A file, and one wants to use the functionality added to the STASHmaster_A in an actual suite, then one needs to make the change like this in 2 places. In fact, when it comes to running the job, one also has to additionally do a manual copy-in of the STASHmaster_A into a sub-directory of the ~/roses/suite-id/app/um/ part of the suite that one wants to run.

So here we need to also do this *manual copy-in* of the updated STASHmaster_A (from either the branch or the metadata directory) into a directory with the particular rose suite you are running.

In fact it's more tricky than that because you actually have to create a new directory called *file* within the app/um/ section of your ~/roses/$SUITE_ID/ file-path and copy-in the updated STASHmaster_A to there. If you don't do this then even though you have updated the STASHmaster_A in the branch, when the model runs it will not use this updated file.

So first you need to cd to ~/roses/$SUITE_ID/app/um and then type *mkdir file*. Then copy the updated STASHmaster_A file from

```
/home/gmann/meta/ga7_vn10.4_MS4updated/etc/stash/STASHmaster/
```

into that new directory you've created called *file*. Even after you've done that, the changes that have been made to the STASHmaster_A will still not be correctly picked up when the job runs until you have added a STASHmaster_A to alert the Rose GUI that this modified STASHmaster_A needs to be *installed* when the model runs. It is regrettable that whereas this was done atuomatically at v8.4 it turns out to be rather cumbersome to do it at v10.4.

Anyway, we need to make an additional change in the Rose GUI to alert the model to the fact that the job needs to use a modified STASHmaster_A file. This is done by adding a new environment variable *STASHMSTR*. Within the *um app* section of the Rose GUI, go to *env* and then select *Runtime Controls*. You see in the right-hand panel it explains this is where environment variables can be set to control behaviour at run time. In our case, this is what we have to do to alert the model that we have changed the STASHmaster_A. It's obviously not ideal that this is not done automatically. But unfortunately that is simply where things are at currently with the new Rose GUI being rolled out before some of the additional functionality is quite ready yet. I expect this will be taken care of at a later UM version but at v10.4 one has to add this extra environment variable to alert the model that things have changed.

So. To add the extra environment variable to alert the model that the STASHmaster_A file has changed. You need to first go to the View panel at the top of the GUI and select *View Latent Variables*. When you have done that you see that there is in fact an entry for specifying the STASHMSTR environment variable. Click on the plus sign next to that STASHMSTR entry and type the single-character string "." into that panel (that's it just the dot). That specifies to pick up the STASHmaster_A from the *file* directory.

Next, I advise to look in the directory src/atmosphere/UKCA of the checked-out branch. This is where all the main UKCA code can be found (including the GLOMAP routines) and also the routines for RADAER, ACTIVATE and FAST-J/JX. The reason I mention this is that I think it is worth taking a look at the routine *ukca_init.F90* as this gives you some idea of how the code processes these different aerosol configurations and how GLOMAP acts on the different settings of I_MODE_SETUP to specify which modes and components are switched ON and OFF. Looking in ukca_init.F90 you see there is the comment that says "Call appropriate MODE setup routine". You see there that, for each different setting for I_MODE_SETUP, the code calls a different trio of "module-procedures" that together set up everything that is needed to run that particular set-up.

If you already know quite a bit about GLOMAP you could take a look at these by looking in the FORTRAN-90 module ukca_mode_setup.F90

In ukca_init.F90 you see that, for I_MODE_SETUP=2, the code specifies to call the module-procedure "ukca_mode_sussbcoc_5mode" whereas for I_MODE_SETUP=4 it calls "ukca_mode_sussbcocso_5mode". These ukca_mode_xxxx routines specify the main logical variables *mode* and *component* which specify which modes are switched on and which components are included in each mode.

The rationale of the GLOMAP setup arrays (set differently in each alternative module-procedure) is that once they are set (along with the associated arrays that specify different properties about each component), the same FORTRAN code can then be run for any supported GLOMAP set-up. For more info about this see the UKCA UMDP (section on GLOMAP aerosol).

The other two *setup indices* module-procedures specify what is done for processes that exchange from the gas phase to the particle phase (principally condensation of *H2SO4* or *SEC_ORG* into one of the aerosol components in the particle modes). The module-procedures set for example how the condensation routine UKCA_CONDEN should direct the condensation from the gas phase into particular components (by direct I mean which component the gas phase should partition into or out of).

Because of the way the code has been written (reasonably flexibly, but note this is only for tried-and-tested GLOMAP set-ups) once these three module-procedures are set, the model then has all it needs to enable the same code to be run with different module-procedures that specify which modes are to be switched on and which off.

At this point, let's get back to the task in hand. Which is to convert your copy of the UKCA tutorial job to run with the two-component POM setup of GLOMAP (I_MODE_SETUP=4).

Now that your suite points to the updated metadata to enable the I_MODE_SETUP=4 GLOMAP setup, and the Rose GUI is all set with the updated STASHmaster_A (including the environment variable STASHMSTR and the manual copy-in of the STASHmaster_A file) things are pretty much ready to go. You just need to add in the extra daily-mean STASH requests for the additional 4 2nd OM mmr's (the SO tracers) as you did to request the standard OM mmrs in task 10. With both sets of OM mmrs requested to the daily-mean .pk files you will be able to validate that there is the same amount of OM in the two-component OM run as in the standard single-component OM run (with also the aerosol optical properties being equivalent).

To add in the extra STASH requests it's just the same procedure as in Task 10 -- go to *Model Input and Output* within the um namelist section of the GUI and then *STASH Requests and Profiles" and then STASH requests*. Click the plus sign next to *New* in the top right-hand corner of the right-hand panel and then add in the section from section 34 items 128, 129, 130 and 131 for the SO mmrs in each of the four soluble modes. To do this double-click on the item so it is added to the list of STASH requests and then set the profile for these 4 new ones as dom_name as *DALLTH* (all theta points in the 3D grid), tim_name as *TDAYM* for daily-mean and use_name as 'UPK' to send these to the .pk files as for the daily-mean OM1 mmrs you already added in Task 10.

Note that whereas at v8.4 the user had to switch to a different version of the RADAER hand-edit *raderv2_vn84_ARCHER.ed* to allow the 2-component OM configuration of GLOMAP to couple to the UM radiation scheme, at v10.4 this is all taken care of automatically within the code (based on the settings for the required user-prognostics in the STASHmaster_A).

So, as the models runs, the AOD's calculated within RADAER will automatically be including the additional partial volume from the OM2 mmr's (items 128 to 131, which now track only the secondary OM) as well as the partial volumes for the usual OC mmrs (which now only include the primary OM).

Finally, since you have asked the model to run with additional tracers, you also need to specify how these should be initialised.

Go to the *Reconfiguration and Ancillary Control* panel in the namelist section of the um app within the Rose GUI and select *Configure ancils and initialise dump fields*. When you select that, the window on the right-hand side should view a whole set of entries which indicate where some of the tracers need a different type of initialisation (not just picking up the values from the dump). These *special initialisations* are handled via what is referred to as an *items namelist*.

The information here is hard to de-cipher but the best way to understand it is to look for the column entitled *stash_req*. That explains which STASH item the panel is specifying needs to be initialised differently. If you click on the *stash_req* it will re-sort the list to be in ascending order for the STASH requests (put section and items in order).

Basically there are several different ways to initialise tracers (or other model fields) when one runs the model. You can specify that they should be set to zero (source set to 3), that they should pick up values from file or *user-ancilliary file* (source set to 7), or else have them be set to a constant (non-zero) value (source set to 6). The UM has been coded to allow the user to specify this very flexibly, based on what is set in the GUI (previously UMUI, now Rose GUI). In short, the choice of how the tracers should be initialised is determined by what is set in the column *source*. If that source column is set to 7 then it means the tracer is to be initiliaised (in an NRUN) by values set in a user-ancilliary file (the name of which is specified in the *ancil filename* column). For example you see that many of the UKCA tracers are set to be initilised from a pre-existing user-ancillary file -- that is set by the environment variable *CHEM_INIT*.

Here, we want to initialise the 4 extra OM2 mmrs to be set to zero at the start of the NRUN so we need to add those in and set them to have the *source* column to be set to 3, for initialising the tracer to zero. To add the extra initialisations you need to right-click in the right-hand window and select *Add section*. You will then get a new row to the column given the index *1*. Then right-click again and select *view namelist items*. This then sets the different items. You need to add all 4 to this one new *section* by, for each one, clicking on section and setting this to section 34 and selecting first 128, then 129, then 130 and then 131 -- clicking on the plus sign after the first one and selecting *Set to zero* from the source section (you only need to do that once). When you add the 2nd one you'll find you need to use the cursor keys due to a bug in the GUI. After clicking Save there will then be an extra line in that list of *special initialisations* which nows list those extra 4 SO mmrs as being initialised to zero.

That's it! With those changes you should be able now to proceed and submit the job as in Task 10.

There is more info in the UMDP on initialising variables in UMDP302:

https://code.metoffice.gov.uk/doc/um/latest/papers/umdp_302.pdf (password required) (https://code.metoffice.gov.uk/doc/um/latest/papers/umdp_302.pdf)

Worked Solution

The worked solution to this task can be found in job **`u-ai897`**. Sample output can be found on ARCHER in the directory

```
/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task11.3
```

Your .pk file should now contain the following fields

```
0    : 192   144   6     1     Unspecified
1    : 192   144   6     1     Unspecified
2    : 192   144   6     1     Unspecified
3    : 192   144   6     1     Unspecified
4    : 192   144   6     1     Unspecified
5    : 192   144   6     1     Unspecified
6    : 192   144   6     1     Unspecified
7    : 192   144   6     1     Unspecified
8    : 192   144   6     1     Unspecified
9    : 192   144   6     1     Unspecified
10   : 192   144   6     1     Unspecified
11   : 192   144   6     1     Unspecified
12   : 192   144   85    1     AITKEN MODE (SOLUBLE) OC MMR
13   : 192   144   85    1     ACCUMULATION MODE (SOL) OC MMR
14   : 192   144   85    1     COARSE MODE (SOLUBLE) OC MMR
15   : 192   144   85    1     AITKEN MODE (INSOLUBLE) OC MMR
16   : 192   144   85    1     NUCLEATION MODE (SOLUBLE) OC2 MMR
17   : 192   144   85    1     AITKEN MODE (SOLUBLE) OC2 MMR
18   : 192   144   85    1     ACCUMULATION MODE (SOLUBLE) OC2 MMR
19   : 192   144   85    1     COARSE MODE (SOLUBLE) OC2 MMR
```

With the exception of the STASHmaster_A file changes, the following Rose edits are required:

```
Index: app/um/rose-app.conf
===================================================================
--- app/um/rose-app.conf        (revision 28536)
+++ app/um/rose-app.conf        (revision 28574)
@@ -1,4 +1,4 @@
-meta=/home/grenville/meta/ga7_vn10.4
+meta=/home/gmann/meta/ga7_vn10.4_MS4updated

 [command]
 default=um-atmos
@@ -23,6 +23,7 @@
 RECON_KEEP_MPP_STDOUT=true
 RECON_STDOUT_FILE=pe_output/${RUNID}.fort6.pe
 SPECTRAL_FILE_DIR=$UMDIR/vn$VN/ctldata/spectral/ga7
+STASHMSTR=.
 UM_THREAD_LEVEL=MULTIPLE
 VN=10.4

@@ -2083,6 +2084,17 @@
 user_prog_ancil_stash_req=34060
 !!user_prog_rconst=1.000000e-12

+[namelist:items(9fcddcd3)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
+source=3
+stash_req=34131
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+!!user_prog_rconst=0
+
 [namelist:items(a01f7039)]
 ancilfilename='$CHEM_INIT_FILE'
 domain=1
@@ -2171,6 +2183,17 @@
 user_prog_ancil_stash_req=34150
 !!user_prog_rconst=0.0

+[namelist:items(aebf9338)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
```

```
+source=3
+stash_req=34130
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+!!user_prog_rconst=0
+
 [namelist:items(af3c6568)]
 ancilfilename=
 domain=1
@@ -2281,6 +2304,28 @@
 !!user_prog_ancil_stash_req=
 user_prog_rconst=1.000000e-18
 
+[namelist:items(d050f041)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
+source=3
+stash_req=34128
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+!!user_prog_rconst=0
+
+[namelist:items(d13ecc0f)]
+ancilfilename=
+domain=1
+!!interval=0
+!!period=1
+source=3
+stash_req=34129
+update_anc=.false.
+!!user_prog_ancil_stash_req=0
+!!user_prog_rconst=0
+
 [namelist:items(dc674670)]
 ancilfilename='$CHEM_INIT_FILE'
 domain=1
@@ -3957,7 +4002,7 @@
 file_strat_aer='Sulfate_SAD_SPARC_Background.asc'
 !!i_mode_bln_param_method=0
 i_mode_nzts=15
-i_mode_setup=2
+i_mode_setup=4
 !!i_so2_hi_level=8
 i_ukca_chem=51
 i_ukca_conserve_method=2
@@ -4110,6 +4155,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'
 
+[namelist:streq(25699046)]
+dom_name='DALLTH'
+isec=34
+item=130
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(26025673)]
 dom_name='DALLTH'
 isec=34
@@ -5870,6 +5923,14 @@
 tim_name='TALLTS'
 use_name='UPUKCA'
 
+[namelist:streq(45fe4ef4)]
+dom_name='DALLTH'
+isec=34
+item=131
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(463b0360)]
 dom_name='DALLTH'
 isec=34
@@ -6206,6 +6267,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'
 
+[namelist:streq(51db0630)]
+dom_name='DALLTH'
+isec=34
+item=128
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(52a891d5)]
 dom_name='DALLTH'
 isec=34
@@ -7750,6 +7819,14 @@
 tim_name='T6HMONM'
 use_name='UPG'

+[namelist:streq(957e3213)]
+dom_name='DALLTH'
+isec=34
+item=129
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(95d040d8)]
 dom_name='DP17'
 isec=30
Index: app/fcm_make_um/rose-app.conf
===================================================================
--- app/fcm_make_um/rose-app.conf       (revision 28536)
+++ app/fcm_make_um/rose-app.conf       (revision 28574)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tropopause_amendment@1
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tropopause_amendment@1
```

These changes (along with the STASHmaster_A file changes) can be found in the file

```
/home/ukca/Tutorial/worked_solutions/Task11.2/task11.2.rose.diff
```

on PUMA.

Task 11.3 Examine the simulated total organic carbon in the original and two-cpt OM configurations

In the above Task 11.2 you ran a 2-component OM version of the UKCA tutorial job (**u-ai071**), which began from the updated version from Task 10 where the AOD diags and the extra STASH requests for OM1 mmrs, had already been added.

You can also refer to the worked solution **u-ai897** which I have configured in this way. See that **u-ai830** was the same as the UKCA tutorial job (with the STASH items from Task 10 added) and then **u-ai897** adds in the required for this Task.

So by now you should have equivalent standard (as **u-ai830**) and 2-component OM (as **u-ai897**) versions of the UKCA tutorial job. In these jobs you have requested numerous daily-mean fields to be output in the .pk files.

So in your /work/n02/n02/ directory on ARCHER you should have **jobid**a.pk19991201 files for your standard and 2-component OM jobs.

Included in the extra STASH requests are the mass mixing ratios of OM (the standard organic component) and SO (the 2nd organic component) in each mode.

The OM mmrs are STASH section 34, items 126 (nucleation mode), 106 (Aitken-soluble), 110 (accumn-soluble), 116 (coarse-soluble) and 121 (Aitken-insoluble).

The SO mmrs are STASH section 34, items 128 (nucleation mode), 129 (Aitken-soluble), 130 (accumn-soluble), 131 (coarse-soluble).

Note that when running with the two-component OM configuration (I_MODE_SETUP=4), the OM mmr in the nucleation mode (34-126) will always be zero, and for that reason the option code in the 4th-from-the-right column in the STASHmaster_A has been set to zero. As a consequence, there will be no 34-126 code available in the .pk file when you run the job.

These STASH item numbers and the details of the standard and 2-component GLOMAP configurations can be found in the UKCA UMDP section 12 Tables 19 and 20.

Note also that there is no SO in the Aitken-insoluble mode as this contains only primary carbonaceous particles. Any SO or OM condensing onto the particles in the insoluble modes is immediately transferred over to the corresponding soluble mode following the "condensation-ageing" approach used by the model. This OM or SO condensing onto the insoluble particles is a kind of "coating" for the particles making the particles hygroscopic/soluble.

You could also try adding STASH requests for the mmr of the gas phase species MONOTER and SEC_ORG (STASH section 34, items 91 and 92).

As an example I have put here a link to a pdf OMcomparison (//www.ukca.ac.uk/wiki/index.php/File:GlobalMap_2cptOM_v104.pdf) showing global maps comparing surface OM fields between the reference single-OM-component suite **u-ai830** (top-left, labelled as `ai830`) and **u-ai895** (top-right, labelled as `ai895`).

Page 1 of the pdf compares the "total POM mmr" at the surface which is the total particulate organic matter (POM) summing up the mass of OM and SO in each mode.

Pages 2 and 3 show comparisons of "total POM1 mmr" and "total POM2 mmr" which are the sum of the 1st and 2nd organic component over all the modes.

You can see from the example that the "total POM2 mmr" in **u-ai830** is zero everywhere. That's because in this job GLOMAP has the standard configuration with just one organic component.

By contrast the "total POM2 mmr" for **u-ai895** has considerable concentrations in vegetated continental regions. In this "I_MODE_SETUP=4" configuration, the "SEC_ORG" species (which contains the secondary organics from monoterpene oxidation) condenses into the "SO" component, whereas in **u-ai830** SEC_ORG condenses into the "OC" component.

The bottom left panel on each page shows a global map of the ratio of the field for the two model runs. One can use this kind of approach to track the fraction of the OM that is biogenic and anthropogenic.

Note however that we initialised the SO mmr's to zero at the start of the 1-day run. So the OC1 mmrs will be spinning down and the SO mmrs will be spinning up. The daily-mean values are averaging over values on each the 1-hour timesteps over which the UKCA chemistry and aerosol processes are integrated. So although the ratio shown in the bottom-left on page 2 is indicative of the biogenic fraction it should be treated with caution as the fields will not have spun-up/down yet.

This task illustrates how one can separate out the aerosol mass from different sources and track them separately via a different aerosol component.

One could also introduce a 2nd gas phase species like "SEC_ORG" to track different types of SOA. For example one could configure the model so that such a 2nd "SEC_ORG2" species held semi-volatile oxidised organic species with only the very low volatility oxidised organics held in the usual "SEC_ORG" species.

Page 4 also confirms there is virtually no difference in simulated AOD between the job that track both types of OM in one component (u-ai830) and the job that has separate components to track primary and secondary OM (u-ai897). The very slight difference apparent in some remote regions (e.g. close to Patagonia), is likely due to differences associated with the so-called *MDTfix* code which protects against artefacts in simulated particle size introduced by mass-conservation imposed in the advection scheme, and corrects slightly differently when the two separate sets of OM tracers are used.

Worked Solution

You can use the following convsh script (or Xconv) to extract the required fields to netCDF:

```
#! /usr/bin/env convsh

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4
# Copyright (C) 2015  University of Cambridge

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# Written by N. Luke Abraham 2017-01-06 <nla27@cam.ac.uk>

# you should change the input file name here
readfile 0 ai922a.pk19880901

# You may need to change the field numbers (first column in Xconv or when using list_fields)
# You should also change the prepended suite-id
# These should match these names:
#  AITKEN MODE (SOLUBLE) OC MMR
writefile netcdf ai922_m01s34i106.nc 12
#  ACCUMULATION MODE (SOL) OC MMR
writefile netcdf ai922_m01s34i110.nc 13
#  COARSE MODE (SOLUBLE) OC MMR
writefile netcdf ai922_m01s34i116.nc 14
#  AITKEN MODE (INSOLUBLE) OC MMR
writefile netcdf ai922_m01s34i121.nc 15
#  NUCLEATION MODE (SOLUBLE) OC2  MMR
writefile netcdf ai922_m01s34i128.nc 16
#  AITKEN MODE (SOLUBLE) OC2 MMR
writefile netcdf ai922_m01s34i129.nc 17
#  ACCUMULATION MODE (SOLUBLE) OC2 MMR
writefile netcdf ai922_m01s34i130.nc 18
#  COARSE MODE (SOLUBLE) OC2 MMR
writefile netcdf ai922_m01s34i131.nc 19
```

You can then use cdo to sum the fields together:

```
cdo add ai922_m01s34i106.nc -add ai922_m01s34i110.nc -add ai922_m01s34i116.nc ai922_m01s34i121.nc ai922_OMmmr_cdo.nc
cdo add ai922_m01s34i128.nc -add ai922_m01s34i129.nc -add ai922_m01s34i130.nc ai922_m01s34i131.nc ai922_SOmmr_cdo.nc
```

You can also use Iris:

```
#!/usr/bin/env python

# This file is part of the UKCA Tutorials:
#  http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorials_at_vn10.4

# Copyright (C) 2015  University of Cambridge

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# version.

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# You find a copy of the GNU Lesser General Public License at <http://www.gnu.org/licenses/>.

# Written by N. Luke Abraham 2017-01-06 <nla27@cam.ac.uk>

# preamble
import iris

# load all OM OC components
om=iris.load('./ai922a.pk19880901',
        [iris.AttributeConstraint(STASH='m01s34i106'),
        iris.AttributeConstraint(STASH='m01s34i110'),
        iris.AttributeConstraint(STASH='m01s34i116'),
        iris.AttributeConstraint(STASH='m01s34i121')])

# load all SO OC components
so=iris.load('./ai922a.pk19880901',
        [iris.AttributeConstraint(STASH='m01s34i128'),
        iris.AttributeConstraint(STASH='m01s34i129'),
        iris.AttributeConstraint(STASH='m01s34i130'),
        iris.AttributeConstraint(STASH='m01s34i131')])

# make cube to store total OM
omsum=om[0].copy()
# make cube to store total SO
sosum=so[0].copy()

# add-up components
omsum.data=om[0].data+om[1].data+om[2].data+om[3].data
sosum.data=so[0].data+so[1].data+so[2].data+so[3].data
```

```
# rename
omsum.rename('mass_fraction_of_total_particulate_organic_matter_in_air')
sosum.rename('mass_fraction_of_total_particulate_organic_matter_in_air')

# remove unlimited dimension when writing to netCDF
iris.FUTURE.netcdf_no_unlimited=True

# output to netCDF
iris.save(omsum,'ai922_OMmmr_iris.nc',netcdf_format='NETCDF3_CLASSIC')
iris.save(sosum,'ai922_SOmmr_iris.nc',netcdf_format='NETCDF3_CLASSIC')
```

The `calc_AOD.py` file provided for the previous Tutorial will also work in exactly the same way here.

These scripts and sample output can be found in the directory

```
/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task11.3
```

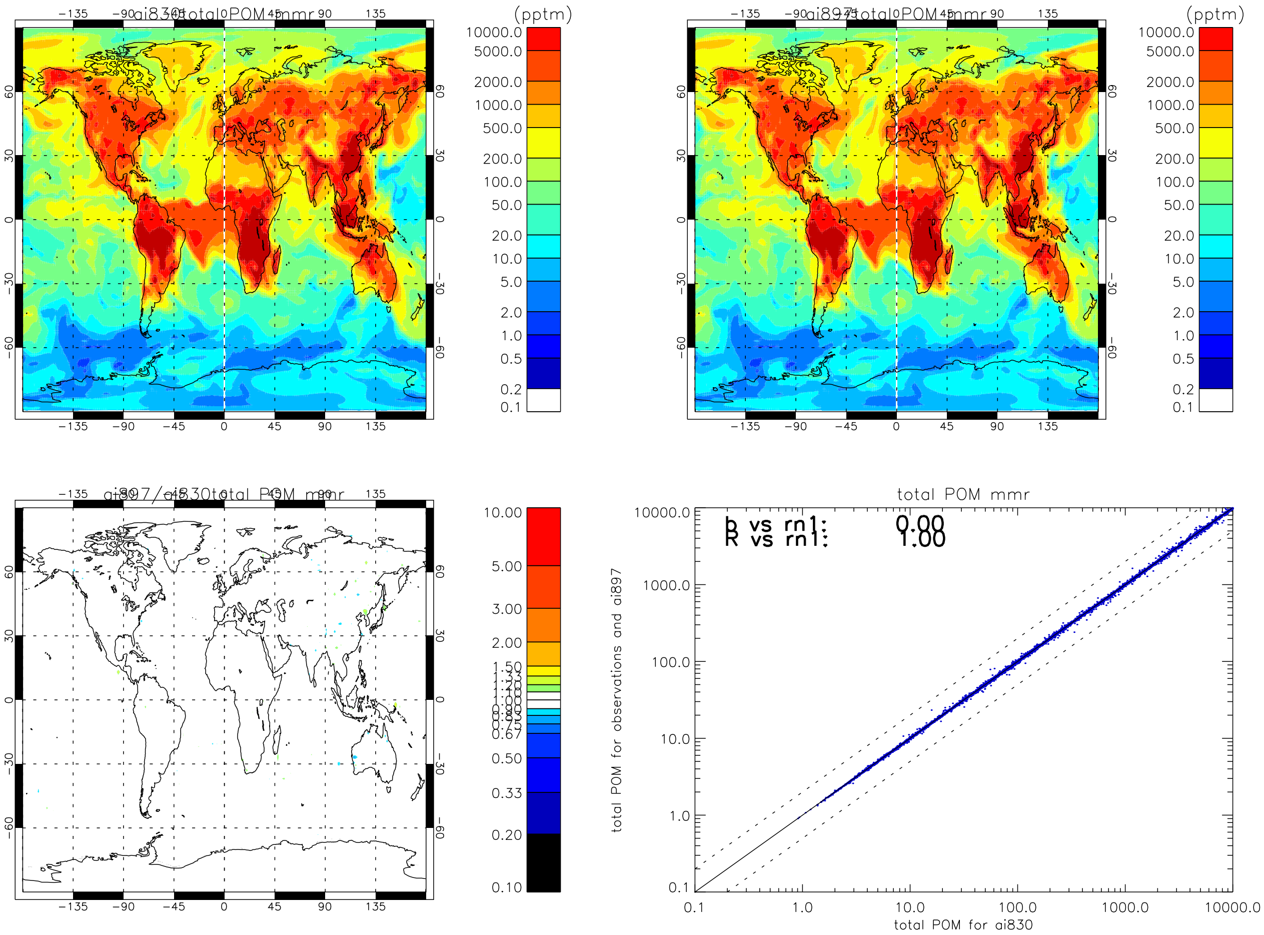
on ARCHER.

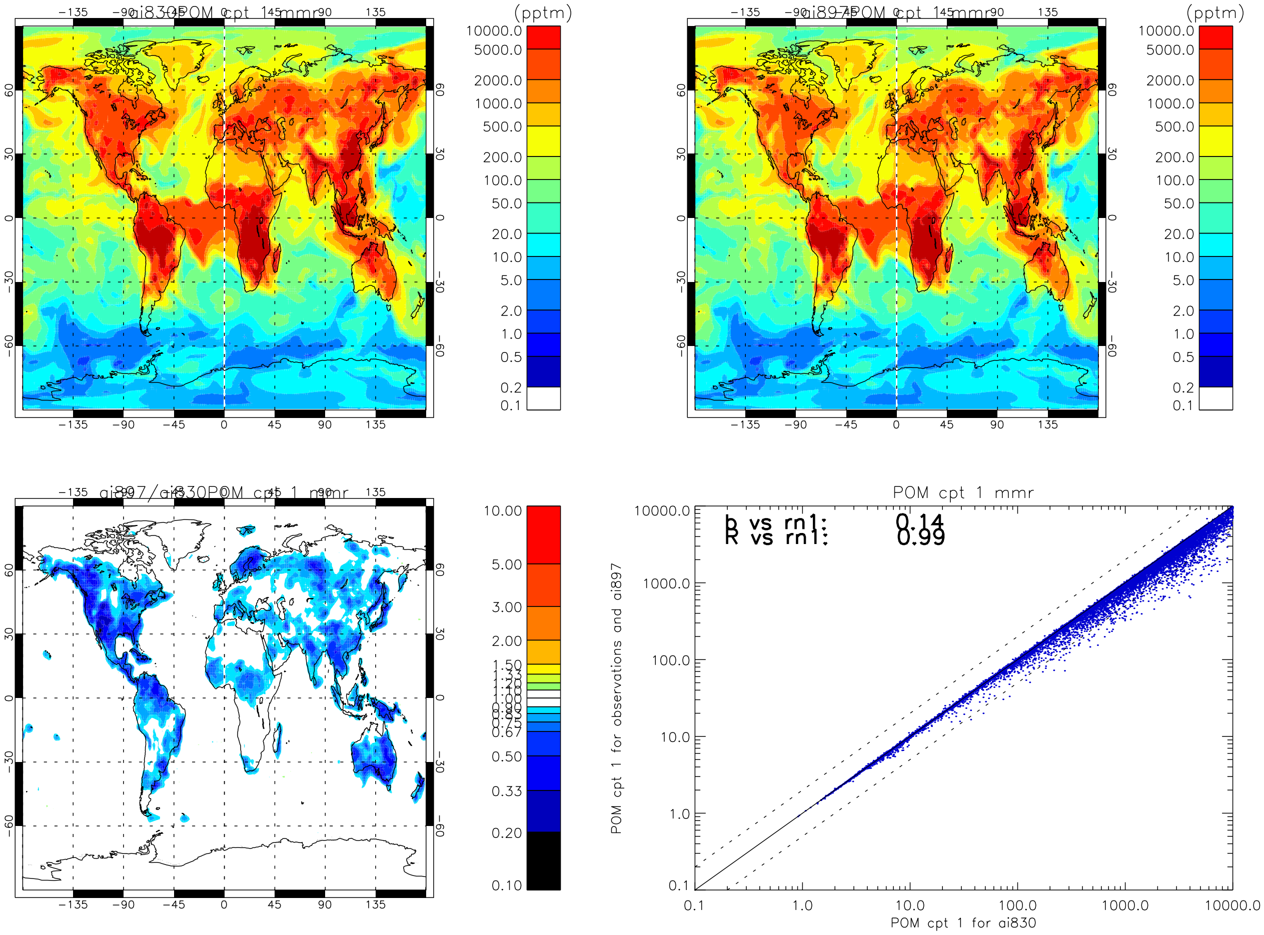
Tutorial 12

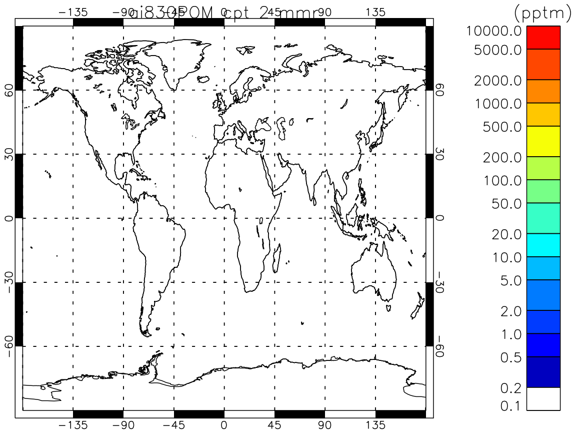
Written by Graham Mann 2016

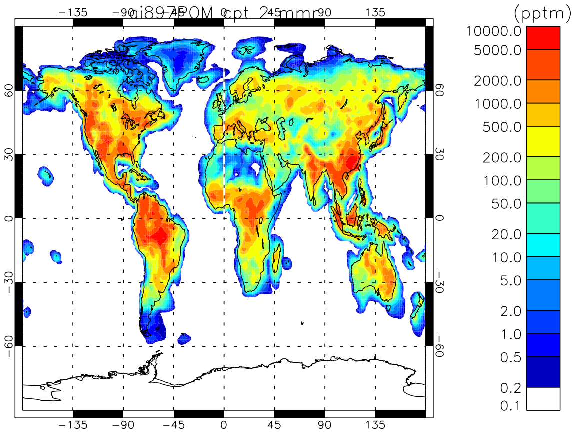
Retrieved from "http://www.ukca.ac.uk/wiki/index.php?title=UKCA_Chemistry_and_Aerosol_vn10.4_Tutorial_11&oldid=5763"

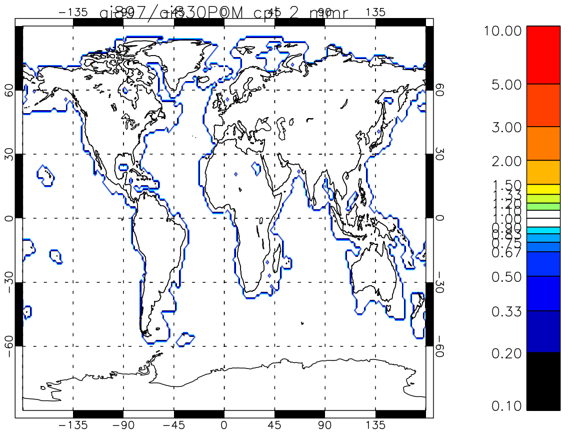
- This page was last modified on 6 January 2017, at 17:31.

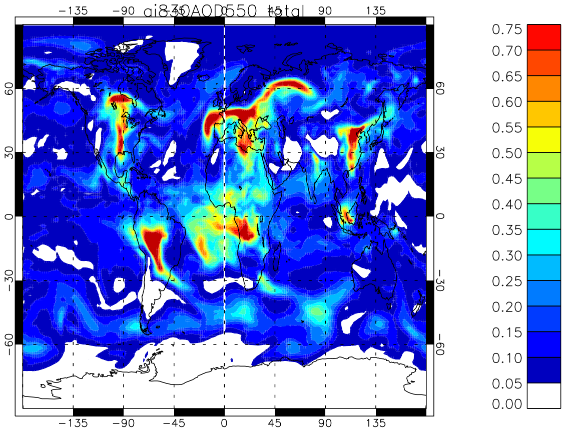

ai830 total POM mmr
(pptm)
10000.0
5000.0
2000.0
1000.0
500.0
200.0
100.0
50.0
20.0
10.0
5.0
2.0
1.0
0.5
0.2
0.1
ai897 total POM mmr
(pptm)
ai897/ai830 total POM mmr
10.00
5.00
3.00
2.00
1.50
1.33
1.20
1.10
1.00
0.90
0.83
0.75
0.67
0.50
0.33
0.20
0.10
-135
-90
-45
0
45
90
135
60
30
0
-30
-60
total POM mmr
b vs rn1: 0.00
R vs rn1: 1.00
total POM for observations and ai897
total POM for ai830
0.1
1.0
10.0
100.0
1000.0
10000.0

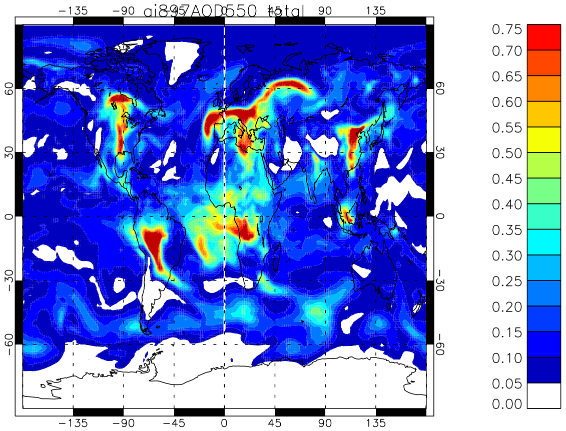

ai830POM cpt 1 mmr
(pptm)
10000.0
5000.0
2000.0
1000.0
500.0
200.0
100.0
50.0
20.0
10.0
5.0
2.0
1.0
0.5
0.2
0.1
-135
-90
-45
0
45
90
135
60
30
0
-30
-60
ai897POM cpt 1 mmr
(pptm)
10000.0
5000.0
2000.0
1000.0
500.0
200.0
100.0
50.0
20.0
10.0
5.0
2.0
1.0
0.5
0.2
0.1
ai897/ai830POM cpt 1 mmr
10.00
5.00
3.00
2.00
1.50
1.33
1.20
1.10
1.00
0.90
0.83
0.75
0.67
0.50
0.33
0.20
0.10
POM cpt 1 mmr
b vs rn1: 0.14
R vs rn1: 0.99
POM cpt 1 for observations and ai897
POM cpt 1 for ai830
0.1
1.0
10.0
100.0
1000.0
10000.0

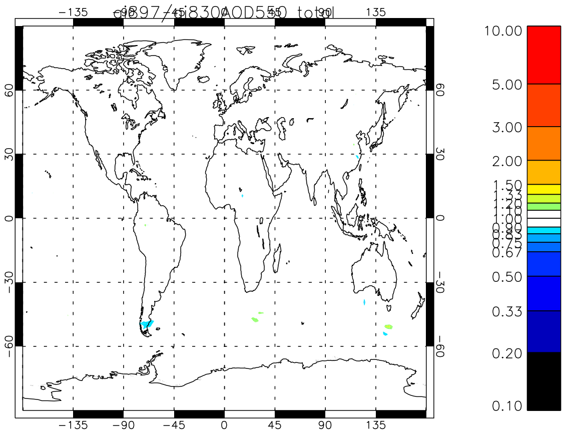

ai830POM cpt 2 mmr
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
(pptm)
10000.0
5000.0
2000.0
1000.0
500.0
200.0
100.0
50.0
20.0
10.0
5.0
2.0
1.0
0.5
0.2
0.1

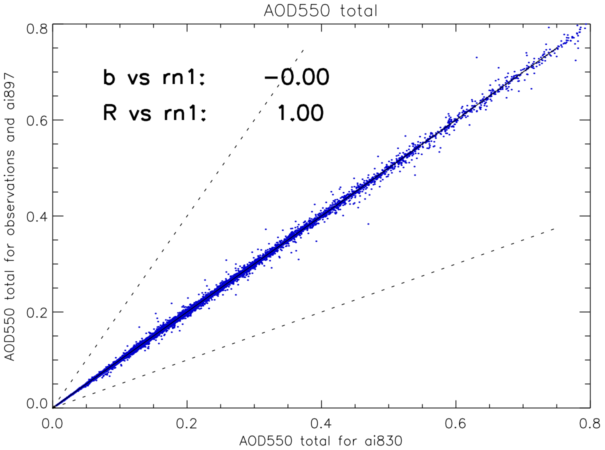

ai897POM cpt 2 mmr
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
(pptm)
10000.0
5000.0
2000.0
1000.0
500.0
200.0
100.0
50.0
20.0
10.0
5.0
2.0
1.0
0.5
0.2
0.1


ai897/ai830POM cpt 2 mmr
−135
−90
−45
0
45
90
135
60
30
0
−30
−60
10.00
5.00
3.00
2.00
1.50
1.33
1.20
1.10
1.00
0.90
0.83
0.75
0.67
0.50
0.33
0.20
0.10


ai830 AOD550 total
-135 -90 -45 0 45 90 135
60 30 0 -30 -60
0.75 0.70 0.65 0.60 0.55 0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00


ai897 AOD550 total
-135 -90 -45 0 45 90 135
60 30 0 -30 -60
0.75 0.70 0.65 0.60 0.55 0.50 0.45 0.40 0.35 0.30 0.25 0.20 0.15 0.10 0.05 0.00


ai897/ai830 AOD550 total
-135 -90 -45 0 45 90 135
60 30 0 -30 -60
10.00 5.00 3.00 2.00 1.50 1.33 1.20 1.10 1.00 0.91 0.83 0.75 0.67 0.50 0.33 0.20 0.10


AOD550 total
b vs rn1: -0.00
R vs rn1: 1.00
AOD550 total for observations and ai897
AOD550 total for ai830
0.0 0.2 0.4 0.6 0.8

UKCA Chemistry and Aerosol vn10.4 Tutorial 12

From UKCA

UKCA Chemistry and Aerosol Tutorials at vn10.4

Contents

What you will learn in this Tutorial

In this tutorial you will learn about how to quantify the radiative effects of aerosol simulated by GLOMAP-mode in UM-UKCA.

In the first task you will update your copy of the UKCA tutorial job to request radiative fluxes allowing the radiative flux perturbation (or effective radiative forcing) to be diagnosed based on difference in the fluxes between a pair of UM-UKCA jobs with some difference (e.g. pre-industrial and present-day emissions jobs).

The second task involves configuring a copy of the UKCA tutorial job to run in *double-call configuration* whereby the aerosol radiative effects can be diagnosed at each radiation timestep.

Task 12.1: Update your copy of the UKCA tutorial job to diagnose Top Of the Atmosphere (TOA) radiative fluxes

In this task you will add STASH requests for SW and LW outgoing radiative fluxes at the top of the atmosphere to enable the radiative forcing from a particular change to be diagnosed.

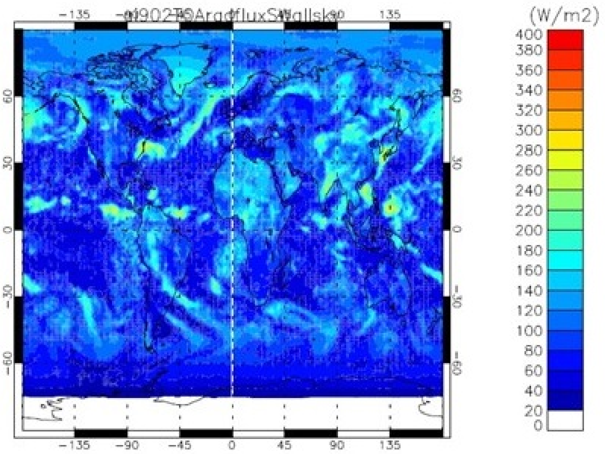
The user should note however that to illustrate the task we are adding these requests to the UKCA tutorial job which is just a 1-day simulation.

One would need to average the flux-difference between the pair of simulations over an appropriate timescale (e.g. multi-annual monthly-means) in order to diagnose an effective radiative forcing appropriately.

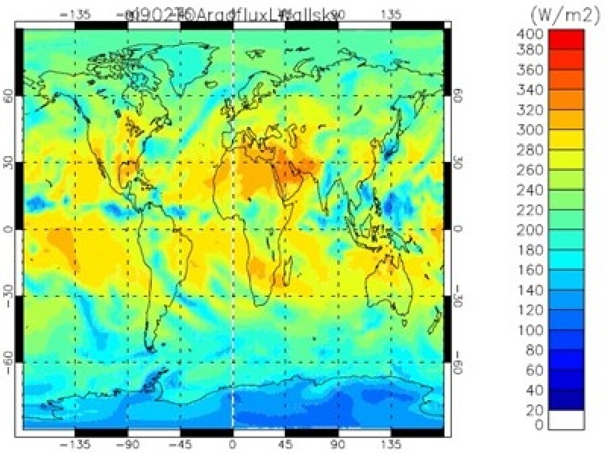
Noting the above caveat, proceed and add daily-mean STASH requests for section 1 item 208 (all-sky outgoing short wave flux at the top-of-the-atmosphere) and section 2 item 205 (all-sky outgoing long wave flux at the top-of-the-atmosphere) to the updated copy of the UKCA tutorial suite you produced in Task 10 after adding AOD and OM diags (the reference job for this is u-ai830).

The radiative fluxes are 2-dimensional diagnostics (longitude by latitude) so you should use the DIAG domain profile in this case. For daily-means use the TDAYM time profile. Again, since we require the daily-mean fluxes to be output to the .pa file you should request the diagnostics with the UPK usage profile.

The Figure below shows the daily-mean SW and LW all-sky TOA radiative flux fields from the UKCA tutorial job for 1st September 1999 (produced by gmann job u-ai902, which updated from u-ai830 by adding in the requests).



Top-Of-the-Atmosphere outgoing Short Wave radiative flux (all-sky)



Top-Of-the-Atmosphere outgoing Long Wave radiative flux (all-sky)

Example Output

You .pk file should now contain the following fields:

```
0    : 192   144   1     1     Upward solar
1    : 192   144   1     1     IR up
2    : 192   144   6     1     Unspecified
3    : 192   144   6     1     Unspecified
4    : 192   144   6     1     Unspecified
5    : 192   144   6     1     Unspecified
6    : 192   144   6     1     Unspecified
7    : 192   144   6     1     Unspecified
8    : 192   144   6     1     Unspecified
9    : 192   144   6     1     Unspecified
10   : 192   144   6     1     Unspecified
11   : 192   144   6     1     Unspecified
12   : 192   144   6     1     Unspecified
13   : 192   144   6     1     Unspecified
14   : 192   144   85    1     AITKEN MODE (SOLUBLE) OC MMR
15   : 192   144   85    1     ACCUMULATION MODE (SOL) OC MMR
16   : 192   144   85    1     COARSE MODE (SOLUBLE) OC MMR
17   : 192   144   85    1     AITKEN MODE (INSOLUBLE) OC MMR
18   : 192   144   85    1     NUCLEATION MODE (SOLUBLE) OC  MMR
```

Example output for Task12.1 can be found on ARCHER in the following directory:

```
/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task12.1
```

The Rose specific changes required are:

```
Index: app/um/rose-app.conf
===================================================================
--- app/um/rose-app.conf        (revision 28624)
+++ app/um/rose-app.conf        (revision 28651)
@@ -6638,6 +6638,14 @@
 tim_name='TRADDM'
 use_name='UPMEAN'

+[namelist:streq(678928ac)]
+dom_name='DIAG'
+isec=1
+item=208
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(67a9602e)]
 dom_name='DIAGAOT'
 isec=2
@@ -8878,6 +8886,14 @@
 tim_name='TDAYM'
 use_name='UPJ'

+[namelist:streq(c8bb6a1f)]
+dom_name='DIAG'
+isec=2
+item=205
+package=
+tim_name='TDAYM'
+use_name='UPK'
+
 [namelist:streq(c8c613fb)]
 dom_name='DALLTH'
 isec=34
```

A file containing these changes can be found at:

```
/home/ukca/Tutorial/worked_solutions/Task12.1/task12.1.rose.diff
```

Task 12.2 Configure the UKCA tutorial job to run as a *double-call* job diagnosing aerosol radiative effects

In this task you will copy the copy of the standard tutorial job you used in Task 12.1 (**u-ai902**) and configure it to run with *double-call* to the radiation scheme to diagnose the radiative effects of the aerosol simulated by GLOMAP in UM-UKCA.

The UM has been coded to allow the user to diagnose radiative effects of a particular forcing agent by calling the radiation scheme twice with one of the calls setting the agent's concentration to zero. Special *forcing* STASH items are included within the UM which store the difference in the radiative fluxes between the two radiation calls.

In the um *app* in the Rose GUI go to namelist --> UM Science Settings and then choose *Section 1 - 2: Radiation.*

In the *General Options* panel, you see that at the top there is an *i_rad_extra_call* "Options for multiple calls to radiation" button-selector.

The UKCA tutorial job is set to "Single call" which is the standard way of running the UM with a single call to the radiation scheme every radiation timestep (here one hour). You see there is a 2nd option there to select "Diagnose radiative forcings". Selecting this option activates the *double-call* approach where the radiation scheme is called twice on each radiation timestep once with the forcing agent and once without it.

With this option, the idea is that the user can then isolate the difference in the radiative fluxes (i.e. the forcing) due to a particular forcing agent of interest. There are a host of additional settings that become available when you select this option setting exactly which forcings to isolate via the difference between the main call and the 2nd call.

The default approach, for this *Diagnose radiative forcings* option, involves the model diagnosing the radiative forcing based on the flux-difference being between the *advancing call* including the radiative effects of the forcing agent (as usual), and the 2nd *diagnostic call* to the radiation setting that species' concentration to zero (or not including its effects in the radiative transfer calculations).

These additional settings for the diagnostic call are set in three of the sub-panels of this *Section 1 - 2: Radiation* part of the Rose GUI. First it can be seen that there are "SW second call" and "LW second call" panels that become active. There is also a separate *Diagnostic forcing* panel for setting the precise arrangement for this second call to the radiation. In this separate panel it is possible to individually (or multiply) select the CLASSIC aerosol types to diagnose their radiative effects. For GLOMAP-mode it's different in that it only makes sense to diagnose the effects over all the types considered since the different types are often internally mixed within each size class. The user will likely only want to run these effects when the settings in the second radiation call match exactly with those in the first radiation call (so that the difference then indicates the forcing due to the forcing agent of interest rather than any difference in settings). If particular experiments are planned, as usual it is recommended to discuss with the relevant expert(s) within NCAS or the Met Office.

As explained above, the default UM setting for the double-call is to set the species mixing ratio to zero in the diagnostic call with the difference then including any fast feedbacks from the forcing agent in the advancing call. However, it is often very useful to be able to suppress the fast feedbacks from the forcing agent in question by reversing the operation of the double-call including the aerosol radiative effects only in the diagnostic call and setting the species mixing ratio to zero in the advancing call.

With this *diagnostic double-call radiative forcing* configuration, the difference in radiative fluxes between the two calls then provides the aerosol radiative perturbation with respect to an atmosphere containing no aerosols. For example, one can diagnose the present-day to pre-industrial aerosol radiative forcing by taking the difference between two parallel diagnostic-double-call simulations with aerosol and precursor emissions set to 1850 and 2000. As long as other forcing agents, such as greenhouse gases or land-use change, remain fixed at a reference time period, the meteorology should then be identical in the two runs, giving a radiative forcing signal "clean" from the different transport arising from the dynamical response to the aerosol radiative effects.

Often nudging to meteorological re-analysis winds and temperatures is applied in tandem with the double-call configuration in which case the composition-climate model is being run in a similar way to an offline chemistry-transport model. This approach has been used extensively in aerosol forcing intercomparisons (e.g. the AeroCom direct forcing experiments, Myhre et al., 2013, ACP) with the radiative forcings diagnosed from each model with fast feedbacks disabled.

Unfortunately, this *diagnostic double-call* configuration is not one of the supported configurations of the v10.4 release job. As a consequence, to run UM-UKCA with this configuration, you will need to add an extra FCM branch to the job and also modify the metadata in the the Rose GUI to enable the option to run configured in this way.

First add the branch. In the fcm_make_um *app* go to *env* and then *Sources.* There you should add an extra entry to add-in the code-changes from revision 32452 of the following FCM branch:

```
branches/dev/grahammann/vn10.4_updates_for_dblcalaerforc@32452
```

The code added in that branch applies a new switch C2C_AER_DIAGCAL which controls whether the setting of the forcing agent to zero is applied on the advancing call (C2C_AER_DIAGCAL is .TRUE.) or to retain the standard operation of the double-call where the aerosol is included in the advancing call but set to zero in the diagnostic call (C2C_AER_DIAGCAL is .FALSE).

We need to use new metadata to enable this switch -- and also to add in a new switch C2C_UKCA_I which controls whether the GLOMAP indirect effects are included or not.

Just like in the last task, this requires to point the Rose GUI to a new rose-meta.conf file within a separate directory outside the FCM branch.

In the Rose GUI click on the *um* word and you'll see that there is already a separate metadata file specified in that job which is set to point to:

```
/home/grenville/meta/ga7_vn10.4
```

I have prepared a modified version of this that enables the extra C2C_AER_DIAGCAL and C2C_UKCA_I switches to be selected in the Rose GUI. So change the file path to instead point to this one:

```
/home/gmann/meta/ga7_vn10.4_dblcalaerforc
```

After you have done this, there will be 2 additional buttons available in the *Diagnostic forcing* panel to allow the user to specify the C2C_AER_DIAGCAL and C2C_UKCA_I switches to be true or false.

We want to use this diagnostic double call configuration and we want to have the forcing be including both the direct and indirect effects from the GLOMAP aerosol -- so set C2C_UKCA_D and C2C_UKCA_I to be .TRUE. You should also set the C2C_DUST_D switch to be true so that the model is then calculating the overall aerosol radiative effects (including both aerosol direct and indirect effects with the aerosol consisting of the total of the 6 CLASSIC dust bins plus the GLOMAP aerosol modes). All the other C2C switches in that panel should be set to .FALSE.

You will also need to update your job to make sure all the settings for the diagnostic call so that they match those set for the prognostic call (in terms of the methods for cloud water content variability, overlapping clouds, and which other forcing agents are interacting (or not).

To check this you should compare the "SW main call" and "SW second call" windows and the "LW main call" and the "LW second call" panels.

Firstly you need to add the *spectral file* name in both second call to match that used in the main call -- see the spectral files used are sp_sw_ga7 for the shortwave and sp_lw_ga7 for the longwave.

Next, select the Shortwave panel and "Number of times per day for full SW radiation calls" is set to 24, which means the radiation scheme is called every hour. The contrasts with the actual model timestep which is set at 20 minutes (see Top Level Model Control --> Model Domain and Timestep). In our double-call case, at every radiation timestep, we want there to be two calls. In other words the frequency for the second SW call needs to be set to match that in the full radiation call. It might seem the user would always want the two to match, but it turns out that in the so-called *single-call timestepping* configuration, this 2nd call is used to enable to call the radiation scheme more frequently but with a reduced operation of the radiation interactions (for details see Manners et al., QJRMS 2009). That's why the first call is referred to as a full call (because in the single-call timestepping configuration the second call is a reduced one. But in our double-call case, the second call is also full and we are diagnosing (on each radiation timestep) the difference to isolate the effects from the forcing agent of interest.

For the Longwave panel, also set the frequency to 24 per day for both.

All that remains then is to add in the extra STASH requests for the double-call forcing diagnostics which give the "increment" (flux-difference) between the two calls and to note a change to the way the AOD diagnostics operate.

The approach taken to index the STASH numbers for the radiative forcing items (the flux-difference between the two radiation calls) is to apply an offset of +200 to the item number to the corresponding item for the conventional radiative fluxes.

In task 12.1 we added STASH requests for the all-sky TOA outgoing SW and LW radiative fluxes which are referenced in STASH as section 1 item 208 and section 2 item 205.

To request the all-sky TOA outgoing SW and LW radiative forcings (between the two radiation calls) the corresponding item numbers are section 1 item 408 and section 2 item 405. Unfortunately however, at UM v10.4, section 2 item 405 is not available from the Rose GUI. In this task we will therefore request instead the clear-sky TOA outgoing SW and LW radiative forcing diagnostics (section 1 item 409 and section 2 item 406). Note also that one needs to request both the radiation flux and radiation forcing diagnostic in these runs so you should add 4 daily-mean STASH requests for section 1 items 209 and 409 and section 2 items 206 and 406.

Go to the *STASH Specification of Diagnostic requirements* window and add the daily-mean (TDAYM) requests for both of these flux-forcing pairs of diagnostics. As in Task 10.1, the domain profile should be set as DIAG and the usage profile as UPK. Note however that the TDAYM time profile is set to sample from the diagnostics on every timestep, whereas in fact these forcing diagnostics are only defined on radiation timesteps. As a consequence, we need to make up a new time profile *TDMN_RAD* which samples every 3 timesteps (on radiation timesteps)) instead of on every timestep. To do this requires to go to *STASH requests and Profiles* and select *Time Profiles*. Again, this is quite an intimidating panel of data, but actually it gives the UM a great deal of flexibility to sample diagnostics during runtime in a myriad of different ways. Here we want to take a copy of the existing TDAYM *time profile* (which calculated daily-means based on the average of values on every timestep) and instead change it to only sample the data every hour (ignoring the values on the other timesteps). You see there is a column in the Table entitled *tim_name* -- this should really be the first column of data because it tells you what the name of the profile is. You see there are profiles such as TDAYMAX -- that takes the maximum value over the day (useful for example in air quality applications for diagnosing exceedance days) and other useful ways of storing some statistics on the data as it is running. This flexibility does potentially make it seem difficult to understand. You can get an idea of what each time profile does by noting its index in the far left column. This number will be in the list underneath. For example the TDAYMAX time profile has the code 3ffa377f. When you then click on that code underneath a panel appears explaining exactly what it does. In our case, we want to take a copy of the TDAYM profile. This is done by right-clicking on the word *TDAYM* in the *tim_name column* and then selecting *Clone this section*. It's confusing because the word *section* is not really correct here -- it should say *profile* not *section*. Still, you know what it means. When you do that it generates a copy of the TDAYM and you should change that name to *TDMN_RAD* and then change the specified frequency of *isam* ("Specify the sampling period (frequency)") to be 3 instead of 1. See it says underneath that the *units* for the sampling period are set as *timesteps*. So we're changing the sampling frequency from once every timestep to once every three timesteps. Once this is done, it's just a case of saving the profile and requesting these double-call radiation diags (1-209, 1-409, 2-206, 2-406) with TDMN_RAD, DIAG and UPK.

Since we have set C2C_AER_DIAGCAL to be .TRUE., when the model runs it will be settings the GLOMAP aerosol to zero in the advancing call. So the conventional AOD diagnostics introduced in tutorial 10 (section 2 items 300 to 305) will now contain zero values when the model is run.

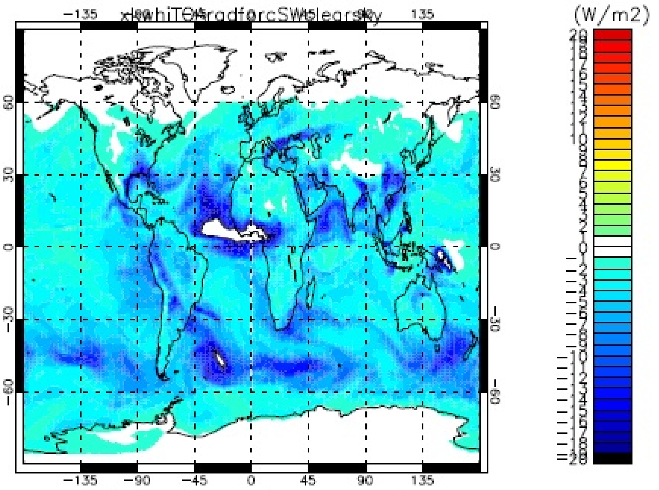
The UM therefore has a second set of AOD diagnostics giving the aerosol optical depth as calculated in the diagnostic call.

The approach for the double-call AOD diagnostics is the same as for the forcing diags, i.e. to apply an offset of +200 to the item number to find the corresponding AOD item in the diagnostic call.

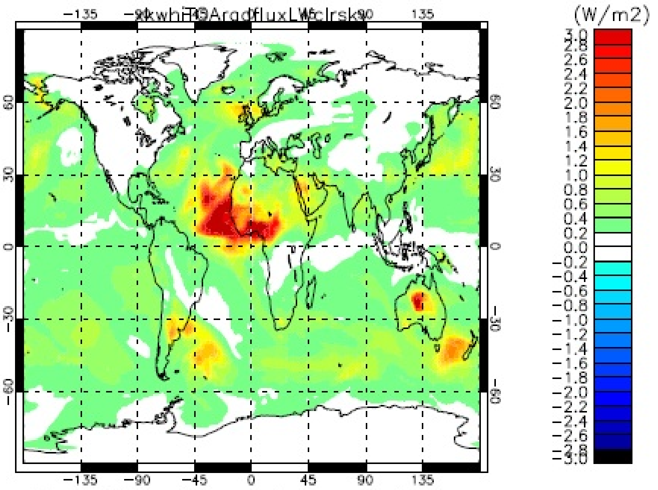
The double-call GLOMAP AOD diagnostics are therefore found in section 2 items 500 to 505. I have added these extra STASH items to the modified STASHmaster_A in the ~gmann/meta/ga7_vn10.4_dblcalaerforc directory that the job is pointing to, so those double-call GLOMAP AODs will be available to select in the Rose GUI. Again, request these with the TDMN_RAD time profile, usage profile UPK and (this time) use domain profile DIAG_AOT (which specifies that 6 pseudo-levels are required for the 6 wavelengths the AODs are calculated for).

The simulation will then output daily-mean SW and LW clear-sky forcings and double-call AOD diagnostics to the .pk file for your v10.4 UM-UKCA job.

The Figure below shows daily-mean TOA SW-clearsky and LW-clearsky radiative effect fields for the double-call-modified version of the UKCA tutorial (gmann job u-ai978).



Top-Of-the-Atmosphere outgoing SW aerosol radiative effect (clear-sky)



Top-Of-the-Atmosphere outgoing LW aerosol radiative effect (clear-sky)

Worked Solution

A worked solution to Task 12.2 can be found in job **u-ai978**.

It should be noted that due to problems with setting up this configuration, the s02i500 to s02i505 fields are corrupted. To prevent the run from failing you need to change the ***packing*** of the .pk file to '**Unpacked (0)**'. This can be done in **um → namelist → Model Input and Output → Model Output Streams → pp10**. With this done the file is created with the fields in place, but it is clear that the diagnostics are corrupted (see Figure 1).

It should be noted that these values may be different in your job. *It is currently unclear why this issue exists, but we hope to fix it soon.*

Sample output from a copy of this job can be found on ARCHER in the directory

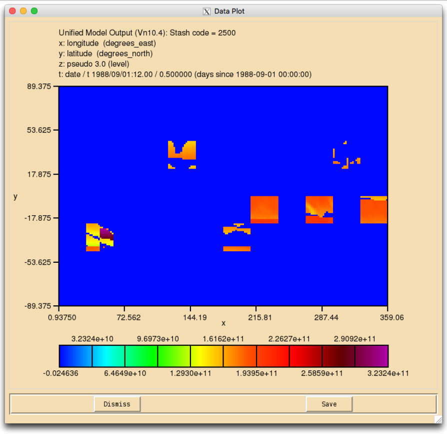
```
/work/n02/n02/ukca/Tutorial/vn10.4/sample_output/Task12.2
```

Your .pk file should contain the following fields:

```
0     : 192   144   1     1      Upward solar
1     : 192   144   1     1      Clear-sky flux (type II) solar up
2     : 192   144   1     1      Clear-sky flux (type II) solar up
3     : 192   144   1     1      IR up
4     : 192   144   1     1      Clear-sky (type II) IR up
```

```
4    : 192   144   1    1    Clear-sky (type II) IR up
5    : 192   144   6    1    Unspecified
6    : 192   144   6    1    Unspecified
7    : 192   144   6    1    Unspecified
8    : 192   144   6    1    Unspecified
9    : 192   144   6    1    Unspecified
10   : 192   144   6    1    Unspecified
11   : 192   144   6    1    Unspecified
12   : 192   144   6    1    Unspecified
13   : 192   144   6    1    Unspecified
14   : 192   144   6    1    Unspecified

15   : 192   144   6    1    Unspecified
16   : 192   144   6    1    Unspecified
17   : 192   144   1    1    Clear-sky (type II) IR up
18   : 192   144   6    1    Unspecified
19   : 192   144   6    1    Unspecified
20   : 192   144   6    1    Unspecified
21   : 192   144   6    1    Unspecified
22   : 192   144   6    1    Unspecified
23   : 192   144   6    1    Unspecified
24   : 192   144   85   1    AITKEN MODE (SOLUBLE) OC MMR
25   : 192   144   85   1    ACCUMULATION MODE (SOL) OC MMR
26   : 192   144   85   1    COARSE MODE (SOLUBLE) OC MMR
27   : 192   144   85   1    AITKEN MODE (INSOLUBLE) OC MMR
28   : 192   144   85   1    NUCLEATION MODE (SOLUBLE) OC  MMR
```



Unified Model Output (Vn10.4): Stash code = 2500
x: longitude (degrees_east)
y: latitude (degrees_north)
z: pseudo 3.0 (level)
t: date / t 1988/09/01:12.00 / 0.500000 (days since 1988-09-01 00:00:00)

Figure 1: m01s02i500, showing the corrupt values.

The Rose specific changes required for this task are (excluding the STASHmaster_A changes):

```
Index: app/um/rose-app.conf
===================================================================
--- app/um/rose-app.conf        (revision 28651)
+++ app/um/rose-app.conf        (revision 28652)
@@ -1,4 +1,4 @@
-meta=/home/grenville/meta/ga7_vn10.4
+meta=/home/gmann/meta/ga7_vn10.4_dblcalaerforc

 [command]
 default=um-atmos
@@ -23,6 +23,7 @@
 RECON_KEEP_MPP_STDOUT=true
 RECON_STDOUT_FILE=pe_output/${RUNID}.fort6.pe
 SPECTRAL_FILE_DIR=$UMDIR/vn$VN/ctldata/spectral/ga7
+STASHMSTR=.
 UM_THREAD_LEVEL=MULTIPLE
 VN=10.4

@@ -2832,7 +2833,7 @@
 !!filename='$ROSE_DATAC/$RUNID.pp10'
 filename_base='$DATAM/${RUNID}a.pk%C'
 l_reinit=.true.
-packing=5
+packing=0
 reinit_end=-1
 reinit_start=0
 reinit_step=90
@@ -3004,140 +3005,142 @@

 [namelist:r2lwclnl]
 i_cnv_ice_lw=8
-!!i_cnv_ice_lw2=8
+i_cnv_ice_lw2=8
 i_cnv_water_lw=5
-!!i_cnv_water_lw2=5
+i_cnv_water_lw2=5
 i_gas_overlap_lw=4
-!!i_gas_overlap_lw2=6
+i_gas_overlap_lw2=4
 i_scatter_method_lw=5
-!!i_scatter_method_lw2=1
+i_scatter_method_lw2=5
 i_st_ice_lw=11
-!!i_st_ice_lw2=8
+i_st_ice_lw2=11
 i_st_water_lw=5
-!!i_st_water_lw2=5
+i_st_water_lw2=5
 l_cfc113_lw=.false.
-!!l_cfc113_lw2=.false.
+l_cfc113_lw2=.false.
 l_cfc114_lw=.false.
-!!l_cfc114_lw2=.false.
+l_cfc114_lw2=.false.
 l_cfc11_lw=.false.
-!!l_cfc11_lw2=.false.
+l_cfc11_lw2=.false.
 l_cfc12_lw=.true.
-!!l_cfc12_lw2=.false.
+l_cfc12_lw2=.true.
 l_ch4_lw=.true.
-!!l_ch4_lw2=.false.
+l_ch4_lw2=.true.
 l_co2_lw=.true.
-!!l_co2_lw2=.true.
+l_co2_lw2=.true.
 l_co_lw=.false.
-!!l_co_lw2=.false.
+l_co_lw2=.false.
 l_cs_lw=.false.
-!!l_cs_lw2=.false.
+l_cs_lw2=.false.
 l_extra_top_lw=.false.
-!!l_extra_top_lw2=.false.
+l_extra_top_lw2=.false.
 l_h2_lw=.false.
```

```
-!!l_h2_lw2=.false.
+l_h2_lw2=.false.
 l_hcfc22_lw=.false.
-!!l_hcfc22_lw2=.false.
+l_hcfc22_lw2=.false.
 l_he_lw=.false.
-!!l_he_lw2=.false.
+l_he_lw2=.false.
 l_hfc125_lw=.false.
-!!l_hfc125_lw2=.false.
+l_hfc125_lw2=.false.
 l_hfc134a_lw=.true.
-!!l_hfc134a_lw2=.false.
+l_hfc134a_lw2=.true.
 l_k_lw=.false.
-!!l_k_lw2=.false.
+l_k_lw2=.false.
 l_li_lw=.false.
-!!l_li_lw2=.false.
+l_li_lw2=.false.
 l_microphysics_lw=.true.
-!!l_microphysics_lw2=.false.
+l_microphysics_lw2=.true.
 l_n2o_lw=.true.
-!!l_n2o_lw2=.false.
+l_n2o_lw2=.true.
 l_na_lw=.false.
-!!l_na_lw2=.false.
+l_na_lw2=.false.
 l_nh3_lw=.false.
-!!l_nh3_lw2=.false.
+l_nh3_lw2=.false.
 l_rb_lw=.false.
-!!l_rb_lw2=.false.
+l_rb_lw2=.false.
 l_solar_tail_flux=.false.
-!!l_solar_tail_flux_2=.false.
+l_solar_tail_flux_2=.false.
 l_tio_lw=.false.
-!!l_tio_lw2=.false.
+l_tio_lw2=.false.
 l_vo_lw=.false.
-!!l_vo_lw2=.false.
+l_vo_lw2=.false.
 spectral_file_lw='sp_lw_ga7'
-!!spectral_file_lw2=
+spectral_file_lw2='sp_lw_ga7'

 [namelist:r2swclnl]
 i_cnv_ice_sw=8
-!!i_cnv_ice_sw2=8
+i_cnv_ice_sw2=8
 i_cnv_water_sw=5
-!!i_cnv_water_sw2=5
+i_cnv_water_sw2=5
 i_gas_overlap_sw=4
-!!i_gas_overlap_sw2=5
+i_gas_overlap_sw2=4
 i_st_ice_sw=11
-!!i_st_ice_sw2=8
+i_st_ice_sw2=11
 i_st_water_sw=5
-!!i_st_water_sw2=5
+i_st_water_sw2=5
 l_ch4_sw=.true.
-!!l_ch4_sw2=.false.
+l_ch4_sw2=.true.
 l_co2_sw=.true.
-!!l_co2_sw2=.true.
+l_co2_sw2=.true.
 l_co_sw=.false.
-!!l_co_sw2=.false.
+l_co_sw2=.false.
 l_cs_sw=.false.
-!!l_cs_sw2=.false.
+l_cs_sw2=.false.
 l_extra_top_sw=.false.
-!!l_extra_top_sw2=.false.
+l_extra_top_sw2=.false.
 l_h2_sw=.false.
-!!l_h2_sw2=.false.
+l_h2_sw2=.false.
 l_he_sw=.false.
-!!l_he_sw2=.false.
+l_he_sw2=.false.
 l_k_sw=.false.
-!!l_k_sw2=.false.
+l_k_sw2=.false.
 l_li_sw=.false.
-!!l_li_sw2=.false.
+l_li_sw2=.false.
 l_n2o_sw=.true.
-!!l_n2o_sw2=.false.
+l_n2o_sw2=.true.
 l_na_sw=.false.
-!!l_na_sw2=.false.
+l_na_sw2=.false.
 l_nh3_sw=.false.
-!!l_nh3_sw2=.false.
+l_nh3_sw2=.false.
 l_o2_sw=.true.
-!!l_o2_sw2=.false.
+l_o2_sw2=.true.
 l_rb_sw=.false.
-!!l_rb_sw2=.false.
+l_rb_sw2=.false.
```

```
 l_solvar_sw=.false.
-!!l_solvar_sw2=.false.
+l_solvar_sw2=.false.
 l_tio_sw=.false.
-!!l_tio_sw2=.false.
+l_tio_sw2=.false.
 l_vo_sw=.false.
-!!l_vo_sw2=.false.
+l_vo_sw2=.false.
 spectral_file_sw='sp_sw_ga7'
-!!spectral_file_sw2=
+spectral_file_sw2='sp_sw_ga7'

 [namelist:radfcdia]
-!!c2c_aerosol=.false.
-!!c2c_all=.false.
-!!c2c_biog_d=.false.
-!!c2c_bmb_d=.false.
-!!c2c_c113=.false.
-!!c2c_cfc11=.false.
-!!c2c_cfc12=.false.
-!!c2c_ch4=.false.
-!!c2c_co2=.false.
-!!c2c_dust_d=.false.
-!!c2c_hcfc22=.false.
-!!c2c_hfc125=.false.
-!!c2c_hfc134=.false.
-!!c2c_land_s=.false.
-!!c2c_n2o=.false.
-!!c2c_nitr_d=.false.
-!!c2c_o3=.false.
-!!c2c_ocff_d=.false.
-!!c2c_seas_d=.false.
-!!c2c_soot_d=.false.
-!!c2c_sulpc_d=.false.
-!!c2c_ukca_d=.false.
-!!c2c_wmg=.false.
+c2c_aer_diagcal=.true.
+c2c_aerosol=.false.
+c2c_all=.false.
+c2c_biog_d=.false.
+c2c_bmb_d=.false.
+c2c_c113=.false.
+c2c_cfc11=.false.
+c2c_cfc12=.false.
+c2c_ch4=.false.
+c2c_co2=.false.
+c2c_dust_d=.true.
+c2c_hcfc22=.false.
+c2c_hfc125=.false.
+c2c_hfc134=.false.
+c2c_land_s=.false.
+c2c_n2o=.false.
+c2c_nitr_d=.false.
+c2c_o3=.false.
+c2c_ocff_d=.false.
+c2c_seas_d=.false.
+c2c_soot_d=.false.
+c2c_sulpc_d=.false.
+c2c_ukca_d=.true.
+c2c_ukca_i=.true.
+c2c_wmg=.false.

 [namelist:recon]
 ainitial='$AINITIAL_N96'
@@ -3743,19 +3746,19 @@
 hfc125mmr=0.0
 hfc134ammr=0
 i_cloud_representation=2
-!!i_cloud_representation_2=2
+i_cloud_representation_2=2
 i_fsd=2
-!!i_fsd_2=0
+i_fsd_2=0
 i_inhom=2
-!!i_inhom_2=0
-!!i_lw_radstep_perday_diag=24
+i_inhom_2=0
+i_lw_radstep_perday_diag=24
 i_lw_radstep_perday_prog=24
 i_overlap=3
-!!i_overlap_2=0
+i_overlap_2=0
 i_ozone_int=2
-i_rad_extra_call=0
+i_rad_extra_call=1
 i_rad_topography=2
-!!i_sw_radstep_perday_diag=24
+i_sw_radstep_perday_diag=24
 i_sw_radstep_perday_prog=24
 inhom_cloud_lw=0
 inhom_cloud_sw=0
@@ -4078,6 +4081,54 @@
 ukcacrsw='$UMDIR/vn$VN/ctldata/UKCA/radaer/nml_cr_sw'
 ukcaprec='$UMDIR/vn$VN/ctldata/spectral/ga7/RADAER_pcalc.ukca'

+[namelist:streq(1)]
+dom_name='DIAGAOT'
+isec=2
+item=500
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
+[namelist:streq(2)]
+dom_name='DIAGAOT'
```

```
+isec=2
+item=501
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
+[namelist:streq(3)]
+dom_name='DIAGAOT'
+isec=2
+item=502
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
+[namelist:streq(4)]
+dom_name='DIAGAOT'
+isec=2
+item=503
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
+[namelist:streq(5)]
+dom_name='DIAGAOT'
+isec=2
+item=504
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
+[namelist:streq(6)]
+dom_name='DIAGAOT'
+isec=2
+item=505
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
 [namelist:streq(00687592)]
 dom_name='DALLTH'
 isec=38
@@ -4966,6 +5017,14 @@
 tim_name='T6HDAYM'
 use_name='UPB'

+[namelist:streq(1fdb379b)]
+dom_name='DIAG'
+isec=1
+item=409
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
 [namelist:streq(200da117)]
 dom_name='DIAG'
 isec=1
@@ -6494,6 +6553,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(5f71be2b)]
+dom_name='DIAG'
+isec=2
+item=406
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
 [namelist:streq(5fb62131)]
 dom_name='DP36CCMZ'
 isec=6
@@ -7790,6 +7857,14 @@
 tim_name='TDMPMN'
 use_name='UPMEAN'

+[namelist:streq(989fcb6a)]
+dom_name='DIAG'
+isec=2
+item=206
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
 [namelist:streq(98ace802)]
 dom_name='DIAG'
 isec=2
@@ -8750,6 +8825,14 @@
 tim_name='TMPMN00'
 use_name='UPMEAN'

+[namelist:streq(c305ce49)]
+dom_name='DIAG'
+isec=1
+item=209
+package=
+tim_name='TDMN_RAD'
+use_name='UPK'
+
 [namelist:streq(c320ea17)]
 dom_name='DIAG'
 isec=2
@@ -10586,6 +10669,25 @@
 !!unt2=2
 unt3=2

+[namelist:time(a8072e80)]
```

```
+!!iedt=0
+iend=-1
+ifre=1
+intv=1
+ioff=0
+iopt=1
+isam=3
+!!isdt=0
+!!iser=0
+istr=1
+!!itimes=0
+ityp=3
+!!lts0=.false.
+tim_name='TDMN_RAD'
+unt1=3
+unt2=1
+unt3=3
+
 [namelist:time(c34e59a7)]
 !!iedt=0
 iend=-1
Index: app/fcm_make_um/rose-app.conf
===================================================================
--- app/fcm_make_um/rose-app.conf       (revision 28651)
+++ app/fcm_make_um/rose-app.conf       (revision 28652)
@@ -45,4 +45,4 @@
 stash_version=1A
 timer_version=3A
 um_rev=vn10.4
-um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tropopause_amendment@19627 branches/dev
+um_sources=branches/dev/mohitdalvi/vn10.4_scale_lightning_nox@19623 branches/dev/stevenhardiman/vn10.4_ukca_tropopause_amendment@19627 branches/dev
Index: rose-suite.conf
===================================================================
--- rose-suite.conf     (revision 28651)
+++ rose-suite.conf     (revision 28652)
@@ -2,7 +2,7 @@
 !!ACCOUNT_USR='foundation'
 ANCIL_OPT_KEYS=
 ARCHER_GROUP='n02-training'
-ARCHER_QUEUE='short'
+ARCHER_QUEUE='standard'
 !!ARCH_LOG=true
 !!ARCH_WALL=true
 ATM_PPN=24
```

These can also be found on PUMA here (including the STASHmaster_A changes):

```
/home/ukca/Tutorial/worked_solutions/Task12.2/task12.2.rose.diff
```

Written by Graham Mann 2016

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