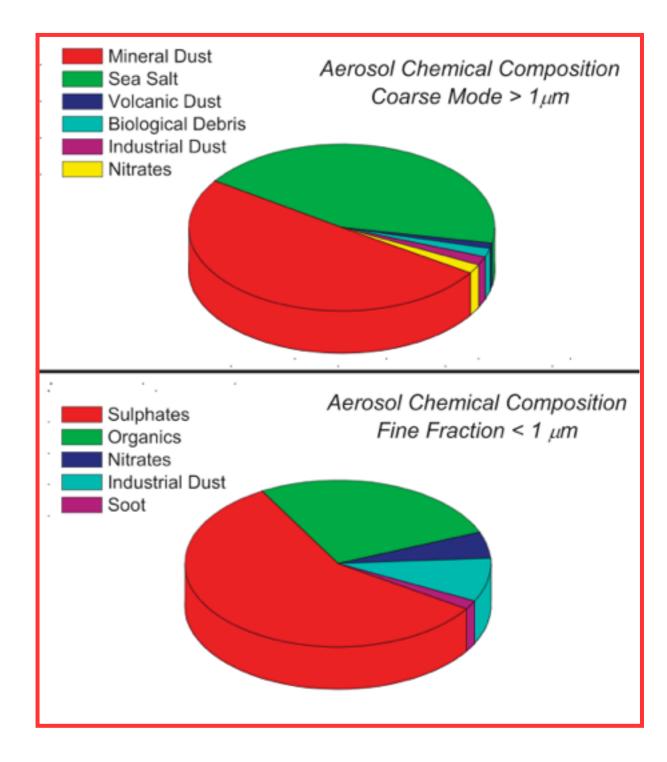
Heterogeneous chemistry - how to get from the literature to UKCA model treatment

Paul Griffiths

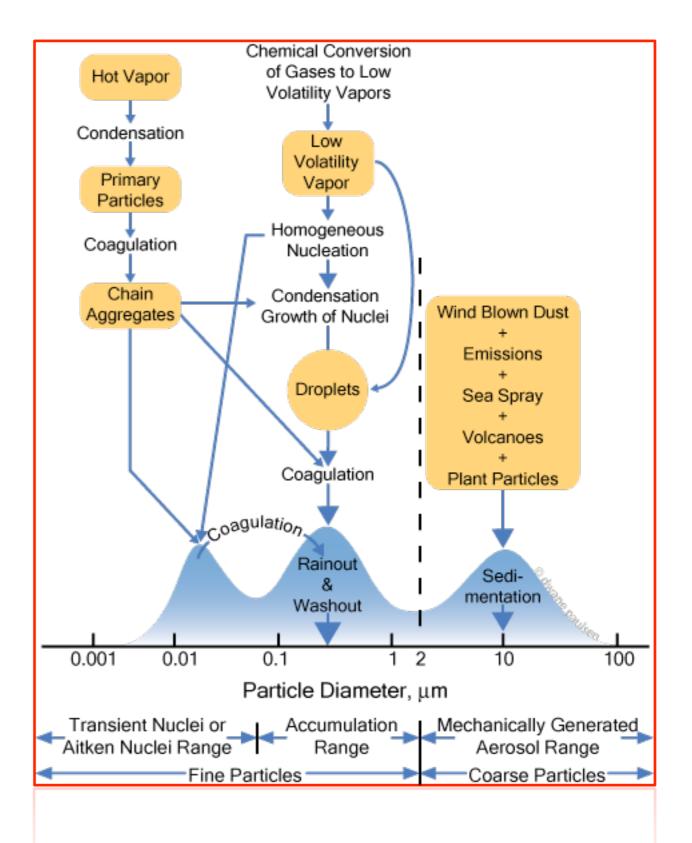
Chemical composition of tropospheric aerosol

- The particulate matter in the atmosphere is very diverse.
- Wide variety of primary sources dust and sea salt are the strongest by mass.
- Chemical transformation of pollutants occurs within the atmosphere, and can lead to aerosol formation.
- $NO_x \rightarrow HNO_3 \rightarrow aerosol nitrate$
- $SO_2 \rightarrow H_2SO_4 \rightarrow \text{ aerosol sulfate}$
- VOC \rightarrow organics (carbon-rich)

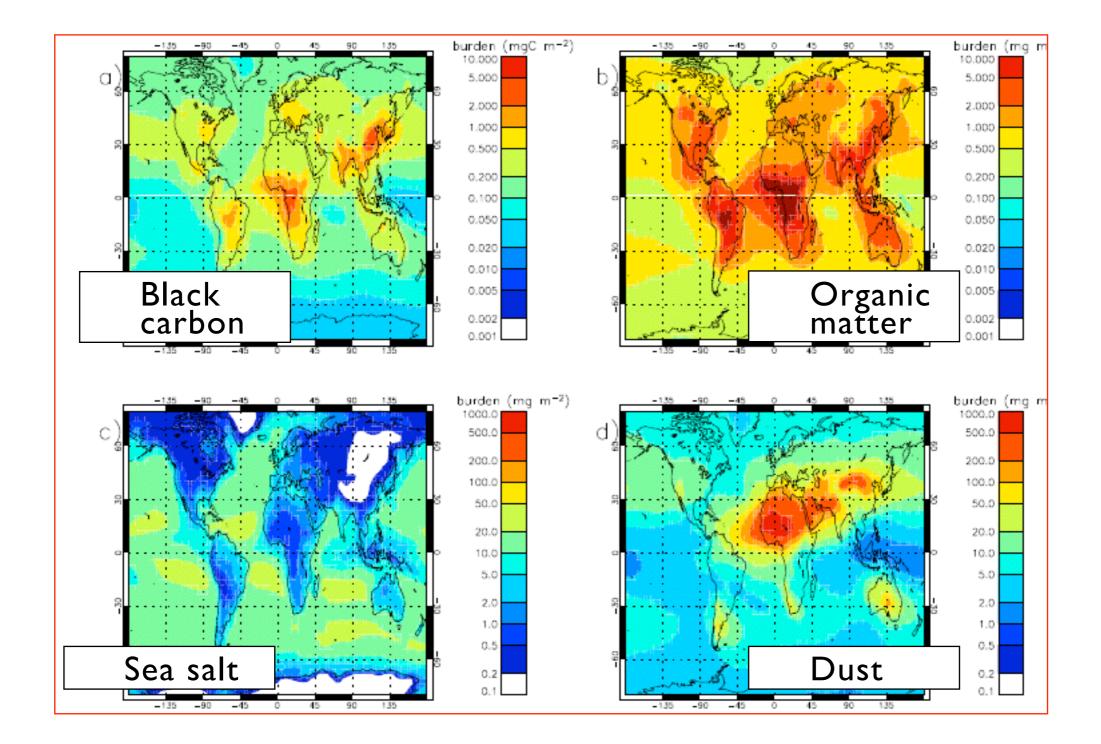


Size range spanned by atmospheric aerosol

- Sizes range from few nm up to hundreds of microns.
- The lifetime of small and large particles is short, but between 100nm and 2 µm, the lifetime can be up to a couple of weeks.
- Dust can be transported across oceans, volcanic aerosol can survive in the stratosphere for years.
- The integrated impact can be large.

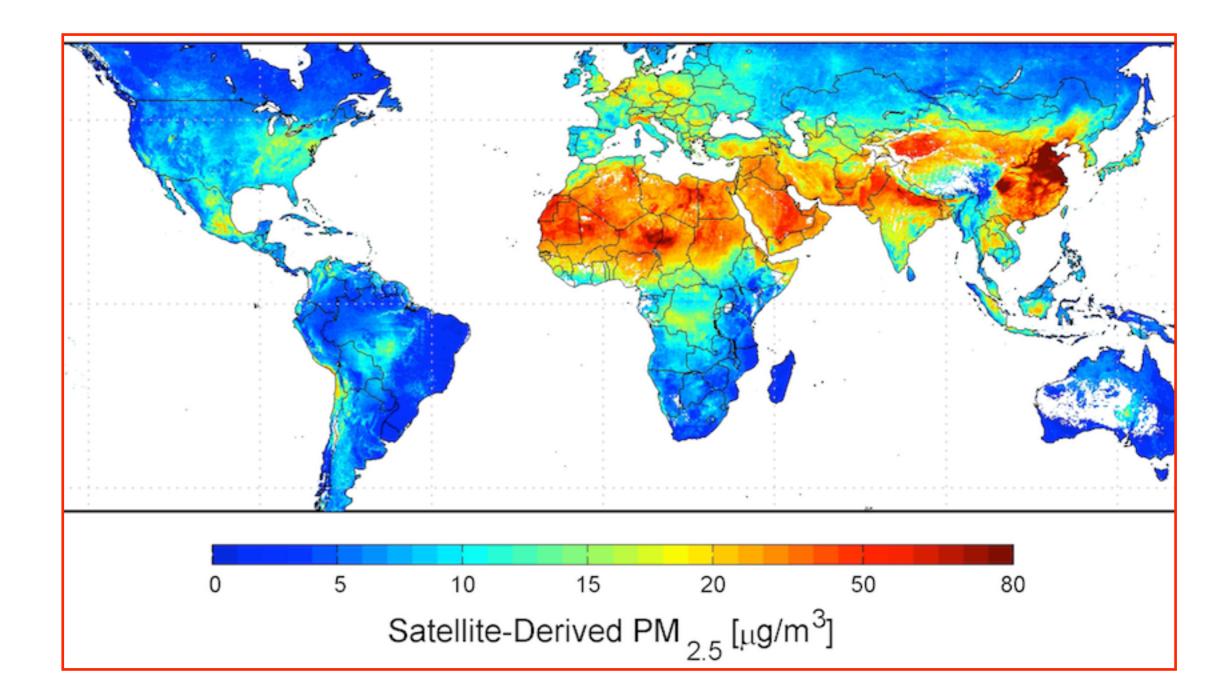


Current work - aerosol chemistry on a global scale



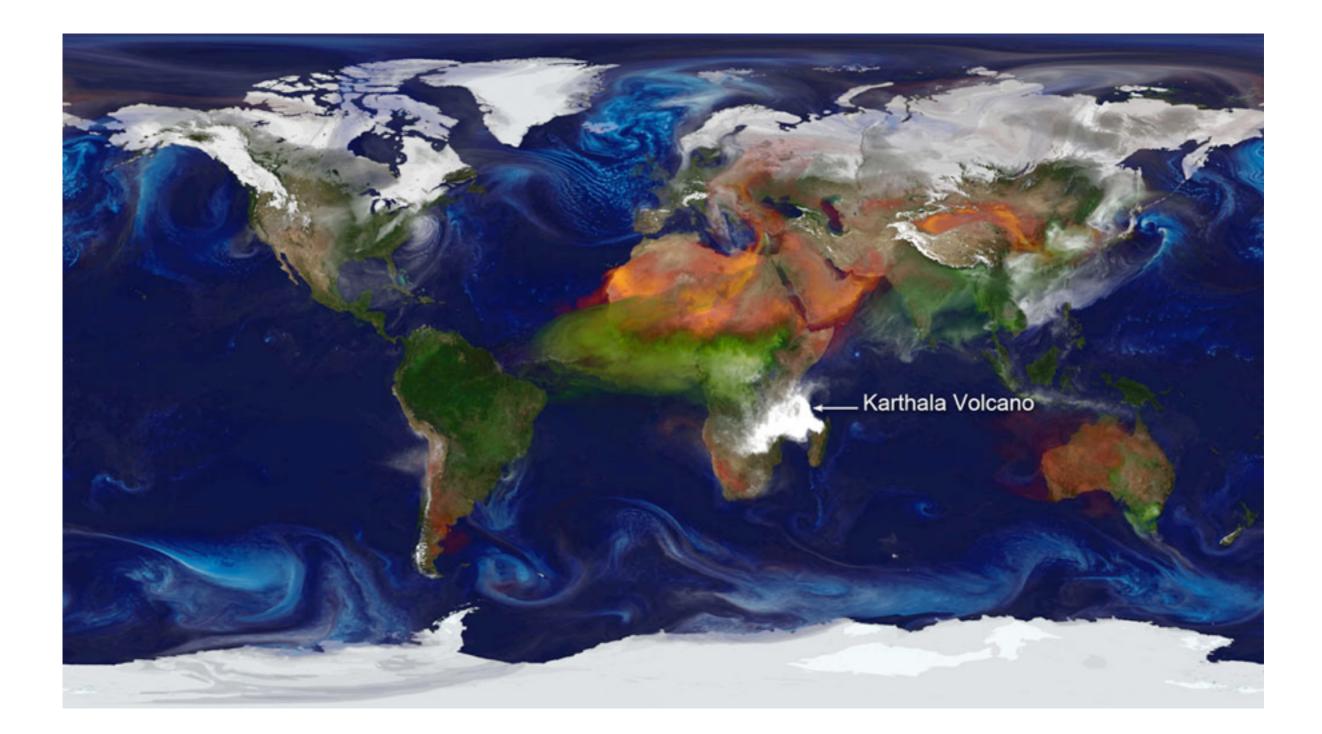
This aerosol model runs within the UK Met Office 'Unified' Climate Model.

Global near-surface distribution of aerosol



Total (mass) particulate matter is shown (NB no measurements over oceans)

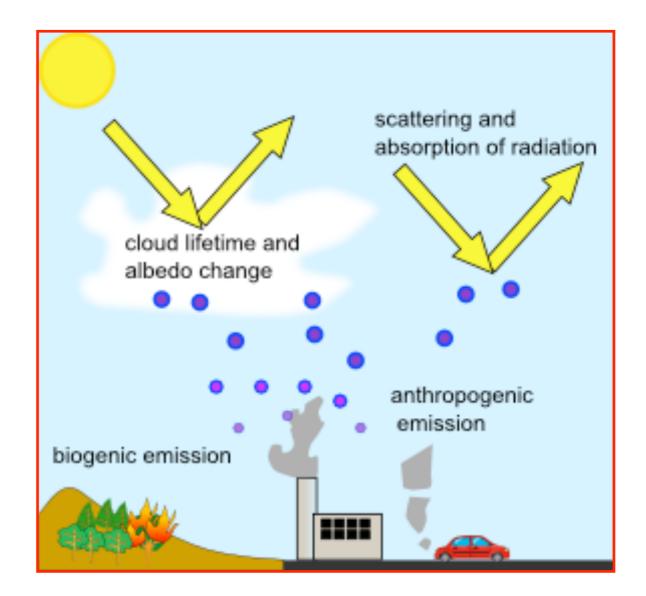
Global distribution of aerosol



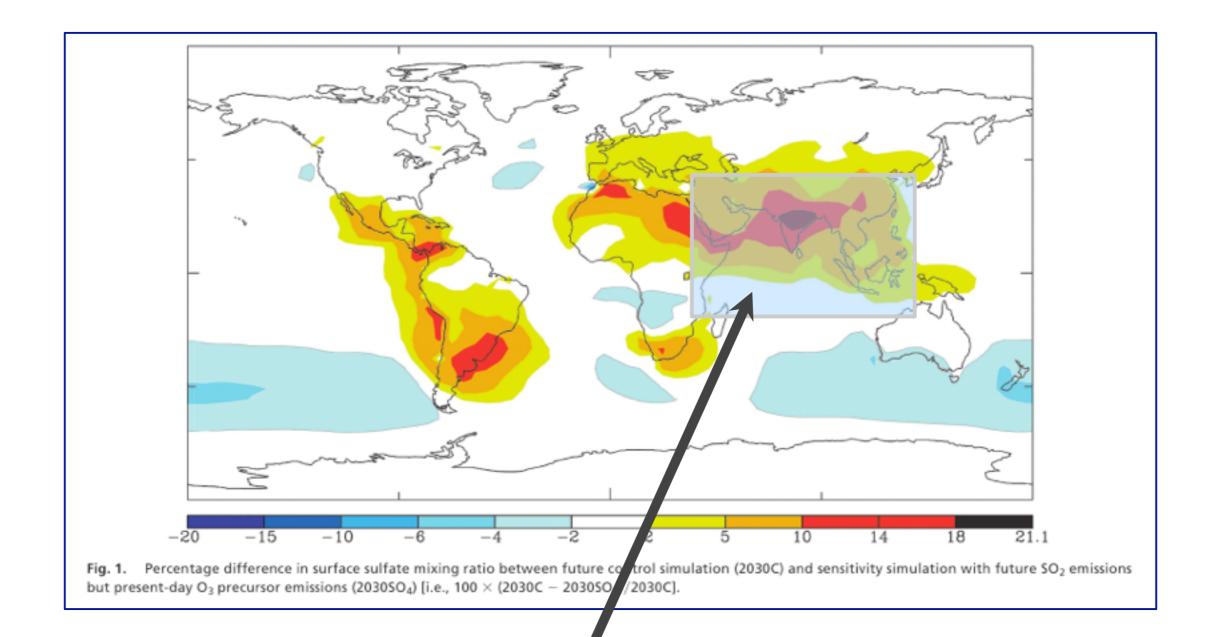
White: sulfate blue: sea salt red: dust green: soot

Aerosols and the chemistry of the troposphere

- Anthropogenic pollutants are degraded by the action of sunlight in the atmosphere to form aerosol.
- Absorption and scattering by the aerosol then change the amount of incident sunlight - local climate different in the neighbourhood of the emissions.
- Also changes the rate of degradation a feedback loop is established.



Coupling between aerosol and oxidation



Regional variations in impact: higher future NOx emissions lead to large increase in [OH], more OH+SO₂, more sulfate. More aerosol means a decrease in solar radiation, moderating climate change.

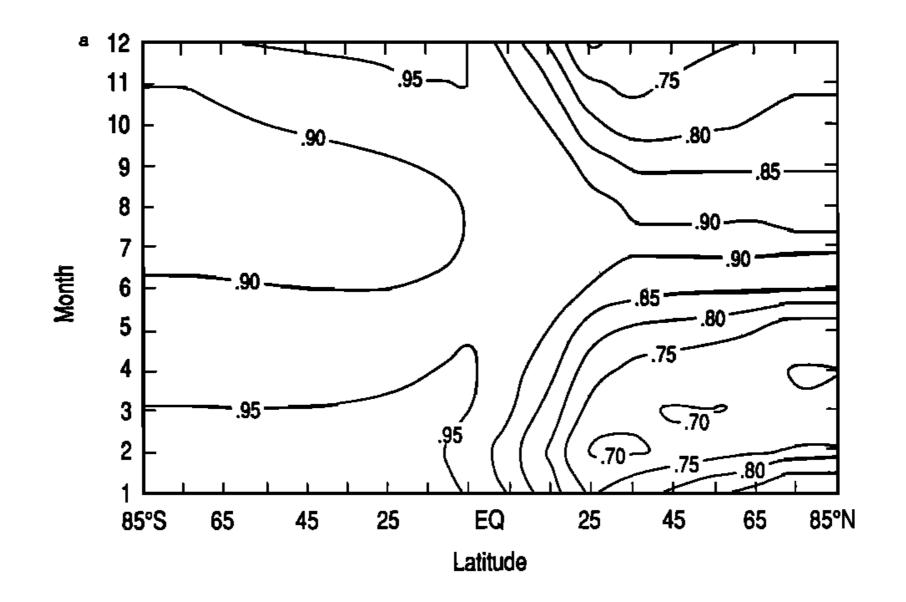


Fig. 9 from Dentener and Crutzen, 1993. The zonal mean monthly average ratio of O3 concentrations with aerosol reactions to those without for all months at 1000 hPa

Particulate matter in the atmosphere

- Serve as the germ or nucleus for cloud formation.
- Scatter incoming solar radiation (reduce heating at the surface).
- Absorb outgoing radiation (increase strength of greenhouse effect).
- Remove (and transform) trace gases and pollutants.
- Health effects

Chemical effects of particles in the atmosphere

- Partitioning to the aqueous phase solubility controlled
- Adsorption onto solid surfaces
- Reactive uptake of trace gases
- Release of trace gases following reactive uptake

• Aerosols may enhance concentration and so open up new pathways of reactivity.

Prognostic equation for reaction of aerosol with gas X

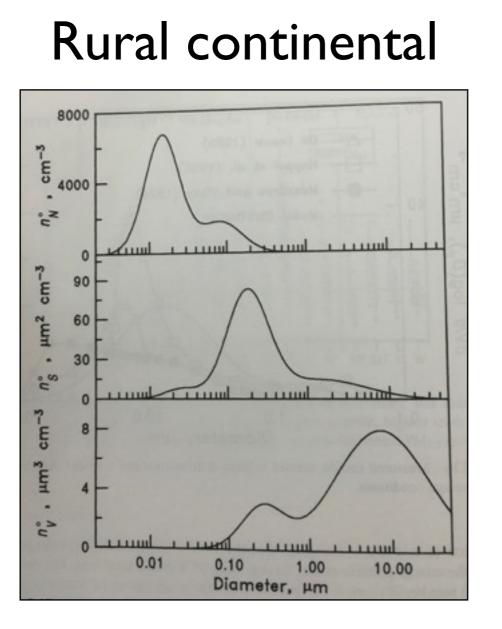
$$\frac{d[X]}{dt} = -k_{het}[X]$$

$$c = \sqrt{\frac{8kT}{\pi m}}$$

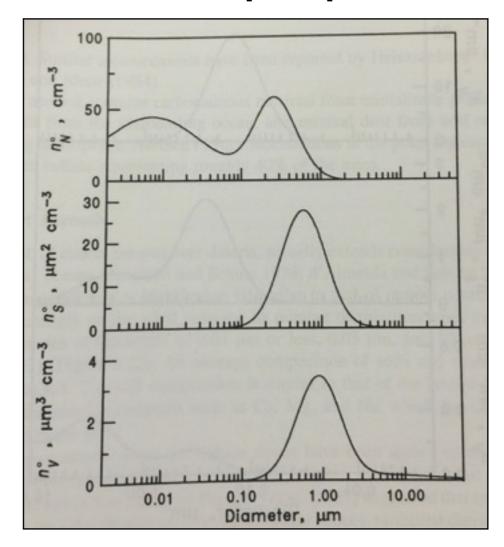
$$k_{het} = \gamma S_a c/4$$

- Parameterise reaction/uptake via uptake coefficient, γ , $(0 < \gamma \le 1)$
- Represents the probability that the gas phase species X is lost per collision with the aerosol surface.
- Make sure units of surface area density (m² m⁻³) and c (mean molecular speed of gas phase X, ms⁻¹) match.
- E.g. typical units of SA density $\mu m^2 m^{-3}$

Representative aerosol number, SA and mass distributions

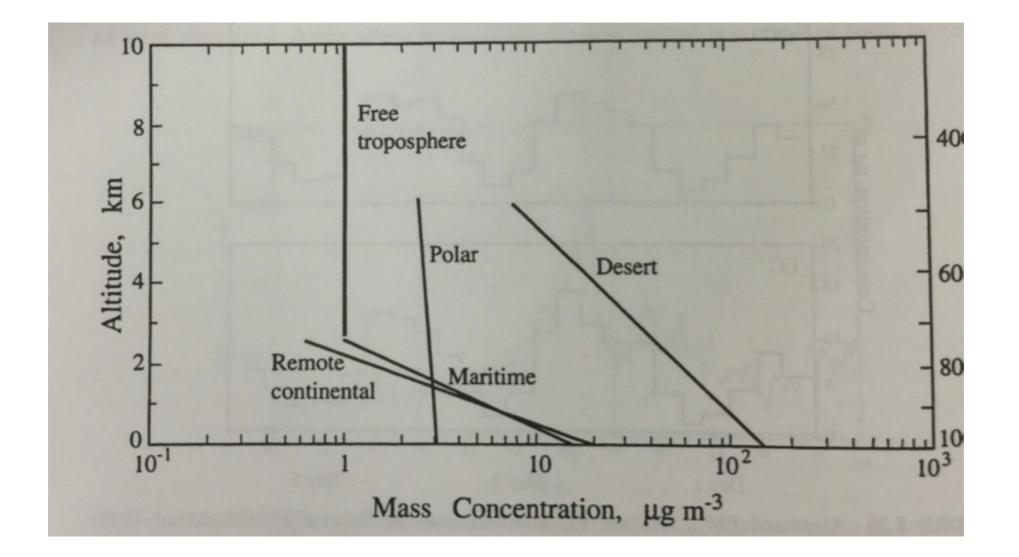


Free troposphere



Maximum of aerosol surface area density is in the accumulation mode

Tropospheric profile of aerosol mass



Figures taken from Seinfeld and Pandis, p. 375

Kinetics of removal of trace gases

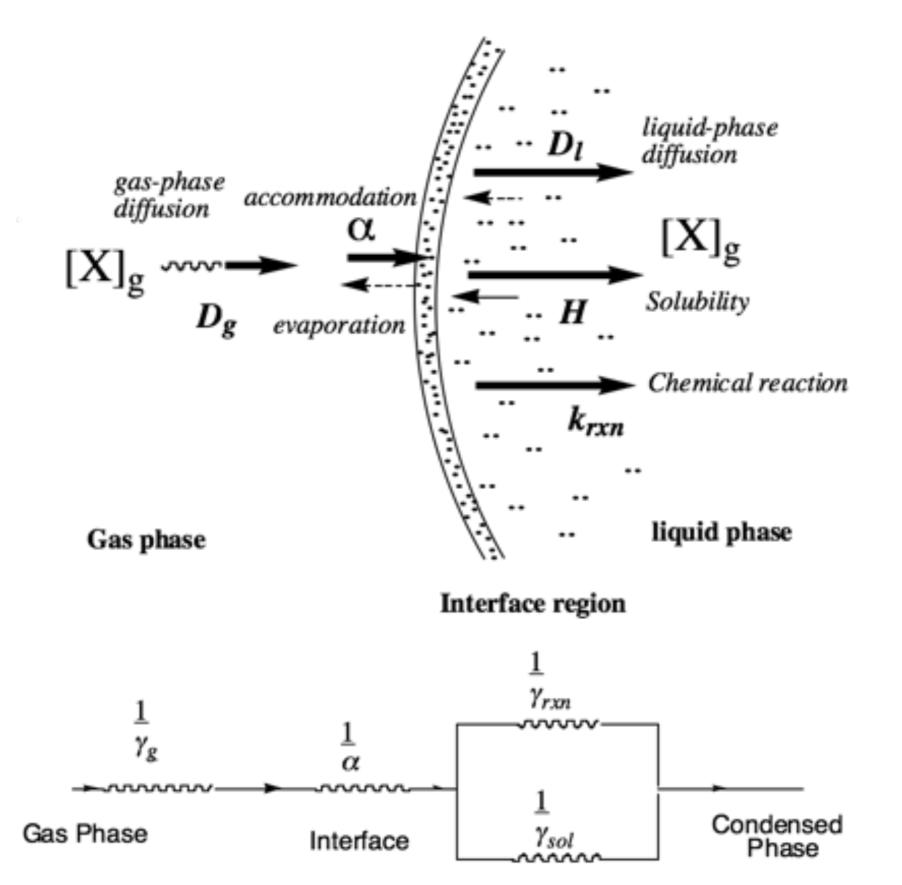
$$\frac{d[X]}{dt} = -k_{het}[X]$$

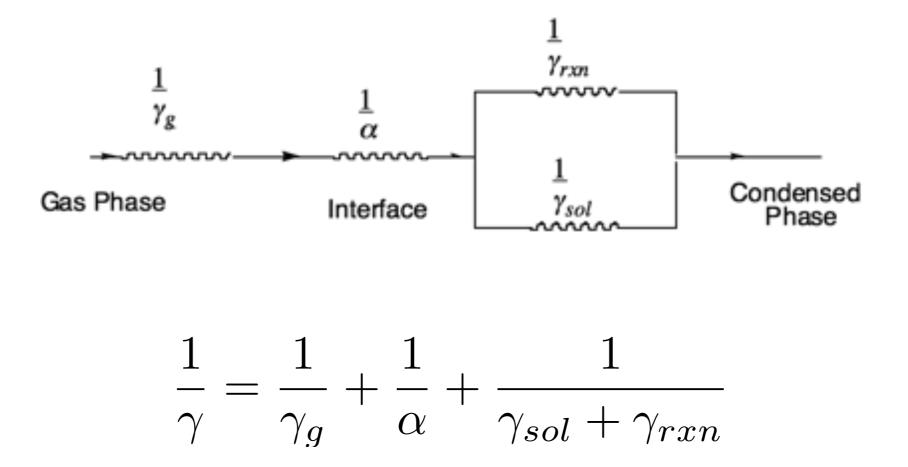
$$c = \sqrt{\frac{8kT}{\pi m}}$$

$$k_{het} = \gamma S_a c/4$$

- The uptake coefficient, γ , contains the physical chemistry that you need to think about.
- This is generally what the experimentalists report.
- Tempting just to take the number from the paper and put it into the model, but there's usually scope to add a bit of value.
- The resistor framework provides the best way currently to do this, although there are other modelling frameworks available e.g. Shiraiwa (PRA framework).

Trace gas uptake by liquids – a series of coupled steps





- The value of gamma can be set by any one of these processes.
- smallest $\gamma \Rightarrow I/\gamma$ dominates sum pays to identify the slowest step!
- If no reaction($\gamma_{rxn} = 0$), then expect the aerosol to become saturated in the trace gas of interest. Over time, the net uptake will reduce to zero.

$$\frac{1}{\gamma} = \frac{1}{\gamma_g} + \frac{1}{\alpha} + \frac{1}{\gamma_{sol} + \gamma_{rxn}}$$

• γ_g represents the modification to the collision frequency (and uptake rate) if the particle is large or diffusion is slow to the particle surface. Depends of particle radius, r, and D_g , gas phase diffusion coefficient

$$\frac{1}{\gamma_g} = \frac{cr}{4D_g}$$

- α is the probability that having collided with the particle surface, the molecule X enters or sticks to the aerosol (NB one way). This can be the smallest probability for solid particles for which this probability is low and so this may control gamma.
- Conversely, when reaction is very fast (γ_{rxn} is large) the accommodation step may again be the slowest step and control γ (so-called 'accommodation-controlled uptake')

$$\frac{1}{\gamma} = \frac{1}{\gamma_g} + \frac{1}{\alpha} + \frac{1}{\gamma_{sol} + \gamma_{rxn}}$$

- γ_{sol} represents the uptake due to the equilibration of the condensed and gas phases establishing a Henry's law equilibrium at which uptake and evaporation are equal - net uptake at this point is zero.
- Key points: that solubility is composition dependent e.g. solubility of SO₂ increases in acidic aerosol; aerosol has probably equilibrated in a UKCA timestep.

$$\frac{1}{\gamma_{sol}} = \frac{\sqrt{\pi}c}{4HRT} \left(\frac{t}{D_l}\right)^{1/2}$$

• Fraction of gas X in aqueous phase can be calculated as

$$\frac{[X_{aq}]}{[X]} = 10^{-6} HRTL$$

• L is liquid water content in g cm⁻³. Can be significant for soluble gases in clouds!

$$\frac{1}{\gamma} = \frac{1}{\gamma_g} + \frac{1}{\alpha} + \frac{1}{\gamma_{sol} + \gamma_{rxn}}$$

- γ_{rxn} represents the uptake due to reaction within the aerosol volume.
- Key points: is composition dependent N₂O₅ onto sulphate (fast) vs nitrate (slow);
 HO₂ onto organic aerosol; O₃ uptake by SOA. Most general form (rarely used)

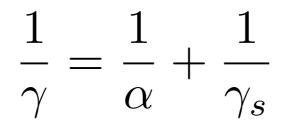
$$\frac{1}{\gamma_{rxn}} = \frac{c}{4HRT\sqrt{D_lk_{rxn}}} \left(\coth q - \frac{1}{q}\right)$$

 krxn is the first-order (s⁻¹) rate constant for loss of X in solution; q is the ratio of particle radius to reacto-diffusive length, l.

$$q = \frac{r}{l} \qquad \qquad l = \sqrt{\frac{D_l}{k_{rxn}}}$$

• In general, the above equation can be simplified.

Uptake onto solid surfaces



- Here reaction is between a surface site or surface bound molecule
- Two limiting cases Langmuir-Hinshelwood (most common by far) or Eley-Rideal
- For Langmuir-Hinshelwood, the reaction is between gas-phase X and a surface-bound molecule Y (here Y_s). Need info on concentration of Y and on partitioning at equilibrium between X and surface-bound X, given by K and N.

$$\frac{1}{\gamma} = \frac{1}{\alpha} + \frac{c(1+K[X])}{4k_{rxn}[Y_s]KN}$$

 For more information see the IUPAC website, <u>http://iupac.pole-ether.fr/htdocs/</u> <u>supp_info/NewHetIntroOct2009.pdf</u>

Back of the envelope

- Need a representative surface area density (or range)
- And a gamma (or range of gammas)
- Then calculate k_{het} for the trace gas of interest
- Compare with other relevant rates e.g. reaction with O₃, dry deposition, wet removal, photolysis, ...
- Can also put into a box model and do an aerosol on/off experiment
 - E.g. KPP http://people.cs.vt.edu/~asandu/Software/Kpp/
 - MECCA http://www.rolf-sander.net/messy/mecca/ mecca_box.html
 - DSMACC <u>https://github.com/barronh/DSMACC</u>

Putting heterogeneous chemistry into UKCA

- Follow the tutorial for putting in a new chemical reaction.
- http://www.ukca.ac.uk/wiki/index.php/UKCA_Chemistry_and_Aerosol_Tutorial_6#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, Fraction of Product 4 produced), &
```

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 (and JPNR)

As with the bimolecular and termolecular reactions, you will also need to increase the values of two parameters that UKCA needs. These are

- JPHK is the number of heterogeneous reactions
- JPNR is the total number of reactions

These are set automatically in the UMUI (depending on what scheme is chosen), and are placed in the &RUN_UKCA namelist in CNTLATM. You will need to make a hand-edit to change these accordingly. The current values can be found by saving and processing the job, and then viewing the CNTLATM file in your \$HOME/umui_jobs/jobid directory.

UKCA/ukca_chem_strattrop.F90

ukca_atriv_mod.F90 428 ratb_t('Monoterp ','03 ','Sec_Org ',' ',',' ', & ukca_atro_tF90 429 ',1.01E-15, 0.00, 732.00, 0.260, 0.000, 0.000, 0.000), & ukca_atro_tF90 439 ratb_t('Monoterp ','N03 ','Sec_Org ',' ',',' ', & ukca_atro_step.F90 431 ',1.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & ukca_be_drydep.F90 431 ',1.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & ukca_be_drydep.F90 433 '',1.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & ukca_be_drydep.F90 433 '',1.19E-12, 0.00, -925.00, 0.260, 0.000,	ukca_abdulrazzak_ghan.F90		
ukca_atron_tF90 429 ' ',1.01E-15, 0.00, 732.00, 0.260, 0.000, 0.000, 0.000), & ukca_arco_tF90 430 ratb_t('Monoterp ','N03 ','Sec_Org ',' ',' ', & ukca_arco_tF90 431 ' ',1.01E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & & ukca_be_drydep.F90 433 ' ',1.01E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & & ukca_be_drydep.F90 433 '' ',0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & & ukca_be_drydep.F90 433 '' ',1.01E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & & ukca_be_drydep.F90 433 '' ',1.01E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & & ukca_be_drydep.F90 433 '' ',1.01E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & & ukca_cher.f90 435 ''' ''''''''''''''''''''''''''''''''''''	ukca_activ_mod.F90		6
ukca_aero_tr90 430 ratb_t('Monterp ','N03 ','Sec_Org ',' ',',',',',',',',',',',',',',',',',	ukca_activate.F90		
disc.garod.pin.g 431 ','.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) & ukca_ageing.F90 432 /) ukca_be_ude.pin.g 433 ','.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & ukca_be_ude.pin.g 433 ','.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & ukca_be_ude.pin.g 433 ','.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000) & ukca_be_ude.pin.g 433 TYPE(RATH_T), ALLOCATABLE :: rath_defs_strattrop_chem(:) & ukca_cla(.oug_kernel.P00 435 TYPE(RATH_T) :: rath_defs_strattrop_psc(1:nhet_strattrop)=(/ & ukca_calc.now_mans.P00 433 rath_t('ClONO2 ','H2O ','HOCl ','HONO2 ',' & & ukca_calcin_maxgc.F00 439 rath_t('ClONO2 ','HCl ','Cl ','Cl ','HONO2 ', & & ukca_calcin_maxindmdt.F00 441 rath_t('HOCl ','HCl ','Cl ','HONO2 ', 'HONO2 ', ', & & ukca_chem_drefs0 443 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ', ', & & ukca_chem_are.F00 444 ', 0.000, 0.000, 0.000, 0.000), & & & ukca_chem_drefs_mod.F00 444 ', 0.000, 0.000, 0.000, 0.000), & & & ukca_chem_are.F00 444 '	ukca_aero_ctl.F90		
diac_losing 432 /) ukca_be_drydep.F90 433 ukca_be_wetdep.F90 433 ukca_be_wetdep.F90 434 ukca_be_wetdep.F90 435 ukca_calc.coag_kernel.F90 435 ukca_calc.coag_kernel.F90 436 ukca_calc.coag_kernel.F90 437 vata_calc.drydiam.F90 437 ukca_calc.ory.zmeans.F90 438 ukca_calc.nov.zmeans.F90 438 ukca_calc.nov.zmeans.F90 439 ukca_calc.nov.zmeans.F90 439 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 442 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 442 ukca_calc.nov.zmeans.F90 441 ukca_calc.nov.zmeans.F90 442 ukca_chem.max.F90 441 ukca_chem.max.F90 442 ukca_chem.ac.F90 444 ukca_chem.ac.F90	ukca_aero_step.F90		
tikac_be_invertep.F90 433 ukca_be_wetdep.F90 434 tikac_abe_invertep.F90 435 tikac_abe_invertep.F90 435 tikac_abe_invertep.F90 435 tikac_abe_invertep.F90 435 tikac_abe_invertep.F90 436 tikac_abe_invertep.F90 437 tikac_abe_invertep.F90 436 tikac_abe_invertep.F90 437 tikac_abe_invertep.F90 438 tikac_abe_invertep.F90 448 tikac_abe_invertep.F90 441 tikac_abe_invertep.F90 443 tikac_abe_invertep.F90 444 tikac_abe_invertep.F90 446 tikac_abe_invertep.F90 446 tikac_abe_invertep.F90 446 tikac_abe_invertep.F90 446 tikac_abe_invertep.F90 448 <td>ukca_aerod.F90</td> <td>431 ',1.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) &</td> <td></td>	ukca_aerod.F90	431 ',1.19E-12, 0.00, -925.00, 0.260, 0.000, 0.000, 0.000) &	
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ukca_binapara_mod.F90 435 ukca_calc_coag_kernel.F90 436 TYPE(RATH_T) :: rath_defs_strattrop_psc(1:nhet_strattrop)=[/ & ukca_calc_drydiam.F90 437 rath_t('ClONO2 ','H2O ','HOCl ','HONO2 ',' ', & ', & ukca_calc_noy_zmeans.F90 438 ' ', 0.0000, 0.0000, 0.0000, & ', 'HONO2 ', ', & ukca_calc_mov_zmeans.F90 438 ' ', 0.0000, 0.0000, 0.0000, & ', 'HCl ','Cl ','HONO2 ', & ukca_calc_minmaxgc.F90 440 ' 0.0000, 0.0000, 0.0000, 0.0000, & ', 'H2O ', 'KL ukca_calc_nucrate.F90 441 rath_t('HOCl ','HCl ','Cl ','HONO2 ',' ', & ukca_chek_md.nd.F90 443 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ',' ', & ukca_chem_ds.F90 444 ' ', 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, & ', 'HONO2 ', ', & ukca_chem_ds.F90 444 ' ', 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, & ', 'HONO2 ', ', & ukca_chem_strg.F90 445 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ','HONO2 ', ', & ', & ukca_chem_std_trop.F90 444 ' ', 0.0000, 0.0000, 0.0000, 0.0000, 0.0000) & ', 'HONO2 ', & ', & ukca_chem_std_trop.F90 445 rath_t('N2O5 ','H2O ','H0NO2 ','H0NO2 ','H0NO2 ', & ', & ukca_chem_std_tro	ukca_be_drydep.F90	433	
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ukca_calc_noy_zmeans.F90 438 '', 0.000, 0.000, 0.000, 0.000), & ukca_calc_pley_diags.F90 439 rath_t('CLONO2 ', 'HCL ', 'CL ', 'HONO2 ', & ukca_calcminmaxgc.F90 440 '', 0.000, 0.000, 0.000, 0.000), & ukca_calcminmaxndmt.F90 441 rath_t('HOCL ', 'HCL ', 'CL ', 'HONO2 ', ' & ukca_calcminmaxndmt.F90 441 rath_t('HOCL ', 'HCL ', 'CL ', 'HONO2 ', ' & ukca_chem.of.F90 442 ' ', 0.000, 0.000, 0.000), & ukca_chem.dr.F90 443 rath_t('N2O5 ', 'H2O ', 'HONO2 ', 'HONO2 ', ' & ukca_chem.dr.F90 444 ' ', 0.000, 0.000, 0.000), & ukca_chem.fat.F90 446 ' ', 0.000, 0.000, 0.000), & ukca_chem.fat.F90 446 ' ', 0.000, 0.000, 0.000), & ukca_chem.fat.F90 447 /)_ ukca_chem.frag.F90 448 ' ukca_chem.frag.F90 450 ! Aerosol chemistry: t	ukca_calc_coag_kernel.F90	436 TYPE(RATH_T) :: rath_defs_strattrop_psc(1:nhet_strattrop)=(/ &	
ukca_clac_plev_diags.F90 439 rath_t('ClONO2 ','HCl ','Cl ','Cl ','HONO2 ', & ukca_calcminmaxgc.F90 440 ', 0.000, 0.000, 0.000), & . ukca_calcminmaxndmdt.F90 441 rath_t('HOCl ','HCl ','Cl ','Cl ','H2O ', & . ukca_calcminmaxndmdt.F90 441 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ',' ', & . ukca_chet_stratloss.F90 443 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ',' ', & . ukca_chet_stratloss.F90 444 ' ', 0.000, 0.000, 0.000), & . ukca_chet_md_ndt.F90 444 ' ', 0.000, 0.000, 0.000), & . ukca_chet_stratloss.F90 444 ' ', 0.000, 0.000, 0.000), & . ukca_chem_loat.F90 445 rath_t('N2O5 ','HCl ','Cl ','NO2 ','HONO2 ', & . ukca_chem_std_trop.F90 446 ' ', 0.000, 0.000, 0.000), & . . ukca_chem_std_trop.F90 447 / . . . ukca_chem_std_trop.F90 448 ukca_chem_strattrop.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products . ukca_chem_strattrop.F90 452 TYPE(RATH_T) :: rath_defs	ukca_calc_drydiam.F90	437 rath_t('ClONO2 ','H20 ','HOCl ','HONO2 ',' ', &	
ukca_calcminmaxgf.F90 440 ' ', 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, 0.000 & ukca_calcminmaxndmdt.F90 441 rath_t('HCL ','HCL ','CL ','H2O ', & ukca_cher_mod.F90 442 ' 0.000, 0.000, 0.000, 0.000, 0.000, 0.000, & ukca_cherk_md_nd.F90 443 rath_t('N2O5 ','H2O ','H0NO2 ','H0NO2 ',' ', & ukca_cherk_md_nd.F90 444 ' 0.000, 0.000, 0.000, 0.000, 0.000, & ukca_cherm_fdat.F90 445 rath_t('N2O5 ','HCL ','CL ','NO2 ','H0NO2 ', ', ukca_chem_arer.F90 446 ' 0.000, 0.000, 0.000, 0.000, 0.000) & ukca_chem_stratfop 448 ' ukca_chem_std_trop.F90 448 ' ukca_chem_stratF90 449 ' ukca_chem_stratF90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_stratfop.F90 451 ! identify the reactions in asad_hetero ukca_chem_stratfop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chem_strg 454 rath_t('SO2 ','NULL0 ',' ',' ', ', & ukca_chem_strg.F90 455 ' 0.0000, 0.000, 0.0000), 0.0000), 0.0000), & &	ukca_calc_noy_zmeans.F90	438 ' ', 0.000, 0.000, 0.000), &	
ukca_calcminmaxgc.F90 440 ' ', 0.000, 0.000, 0.000, 0.000), & ukca_calcminmaxndmdt.F90 441 ' rath_t('HCl ','HCl ','Cl ','H2O ','H2O ','BACO', & ukca_calcnucrate.F90 442 ' 0.000, 0.000, 0.000, 0.000), & ukca_chef_stndtoss.F90 443 ' rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ',' ', & ukca_chem_acr.F90 444 ' 0.000, 0.000, 0.000, 0.000), & . ukca_chem_daf.F90 445 ' rath_t('N2O5 ','HCl ','Cl ','NO2 ','HONO2 ', ', & ukca_chem_acr.F90 446 ' 0.0000, 0.000, 0.0000, 0.000), & . ukca_chem_acr.F90 446 ' 0.0000, 0.000, 0.0000, 0.0000, 0.0000), & . ukca_chem_acr.F90 446 ' 0.0000, 0.000, 0.0000, 0.0000, 0.0000, & . ukca_chem_acr.F90 447 / . . ukca_chem_strd_trop.F90 448 . . . ukca_chem_strd_trop.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_strat.F90 451 ! identify the reactions in asad_hetero . ukca_chemco.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco.F90 453 <t< td=""><td>ukca_calc_plev_diags.F90</td><td>439 rath_t('ClONO2 ','HCl ','Cl ','Cl ','HONO2 ', &</td><td></td></t<>	ukca_calc_plev_diags.F90	439 rath_t('ClONO2 ','HCl ','Cl ','Cl ','HONO2 ', &	
ukca_calcminmaxndmdt.F90 441 rath_t('HOCl ','HCl ','Cl ','Cl ','H2O ', & ukca_calcnucrate.F90 442 ' ', 0.000, 0.000, 0.000, 0.000, 0.000), & ukca_chd_stratloss.F90 443 rath_t('N2O5 ','H2O ','HONO2 ','HONO2 ',' ', & ukca_chek_stratloss.F90 444 ' ', 0.000, 0.000, 0.000, 0.000), &	ukca_calcminmaxgc.F90		
ukca_calcnucrate.F90 442 ' ', 0.000, 0.000, 0.000, 0.000), & ukca_cdnc_mod.F90 443 rath_t('N205 ','H20 ','H0N02 ','H0N02 ',' ', & ukca_ched_stratioss.F90 444 ' ', 0.000, 0.000, 0.000), 0.000), & ukca_check_md_nd.F90 445 rath_t('N205 ','HCl ','Cl ','N02 ','H0N02 ', 'H0N02 ', ' ukca_chem_idef.F90 446 ' ', 0.000, 0.000, 0.000), 0.000), & ukca_chem_aer.F90 446 ' ', 0.000, 0.000, 0.000), 0.000), & ukca_chem_aer.F90 447 /) ukca_chem_staf_trop.F90 448 ukca_chem_staf_trop.F90 449 ukca_chem_strat.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_staf_trop.F90 451 ! identify the reactions in asad_hetero ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco_raq.F90 453 !HS03+H202(aq) ukca_chemistry.tl.F90 455 ', 0.0000, 0.0000, 0.0000), 0.0000), 0.0000), . &	ukca_calcminmaxndmdt.F90		
ukca_cdnc_mod.F90 443 rath_t('N205 ','H20 ','H0N02 ','H0N02 ',' ', ', & ukca_ch4_stratloss.F90 443 rath_t('N205 ','H20 ','H0N02 ','H0N02 ',' ', & ukca_check_md_nd.F90 444 ', 0.0000, 0.0000, 0.0000, 0.0000), & ukca_chem_ldat.F90 445 rath_t('N205 ','HCl ','Cl ','N02 ','H0N02 ',' & ukca_chem_arer.F90 446 ', 0.0000, 0.0000, 0.0000, 0.0000) & ukca_chem_ater.F90 447 /) ukca_chem_strat.F90 448 ukca_chem_strat.F90 449 ukca_chem_strat.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_strat.F90 451 ! identify the reactions in asad_hetero ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ ukca_chemco_F90 453 !HS03+H202(aq) ukca_chemco_raq.F90 454 rath_t('S02 ', 'NULL0 ',' NULL0 ',' ',' ', & ukca_chemistry_ctl.F90 455 ', 0.0000, 0.0000, 0.0000), 0.0000), 0.0000), &	ukca_calcnucrate.F90		
ukca_ch4_stratloss.F90 444 ' ', 0.000, 0.000, 0.000, 0.000), & ukca_chem1_dat.F90 445 rath_t('N2O5 ','HCl ','NO2 ','HONO2 ', & ukca_chem_aer.F90 446 ' ', 0.000, 0.000, 0.000) & 446 ','O.000, 0.000, 0.000) & ukca_chem_aer.F90 446 ' ', 0.000, 0.000, 0.000) & 447 /) ukca_chem_strad.F90 448 ' '/ '/ 448 ukca_chem_strat.F90 449 ' '/ '/ ukca_chem_strat.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_strattrop.F90 451 ! identify the reactions in asad_hetero ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco.r40 453 !HS03+H202(aq) ' ', 0.0000, 0.000, 0.0000), . & ukca_chemistry_ctl.F90 455 ' ', 0.0000, 0.0000, 0.0000), . & &	ukca_cdnc_mod.F90		
ukca_check_md_nd.F90 445 rath_t('N205 ','HCl ','Cl ','N02 ','HON02 ', & ukca_chem1_dat.F90 446 ', 0.0000, 0.0000, 0.0000, 0.0000) & ukca_chem_aer.F90 446 ', ', 0.0000, 0.0000, 0.0000) & ukca_chem_strat.F90 447 /)_ ukca_chem_strat.F90 448 ukca_chem_strat.F90 450 ! Aerosol chemistry: there are no gas phase products, the 'NULLx' products ukca_chem_strattrop.F90 451 ! identify the reactions in asad_hetero ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco_raq.F90 454 rath_t('S02 ','H202 ','NULL0 ',' ', & ukca_chemistry_ctl.F90 455 ' ', 0.0000, 0.0000, 0.0000), 0.0000), 0.0000), . & &	ukca_ch4_stratloss.F90		
ukca_chem1_dat.F90 446 ' ', 0.000, 0.000, 0.000) & ukca_chem_aer.F90 447 //_ ukca_chem_defs_mod.F90 448 /_ ukca_chem_std_trop.F90 449	ukca_check_md_nd.F90		
ukca_chem_aer.F90447//ukca_chem_defs_mod.F90447//ukca_chem_std_trop.F90448ukca_chem_std_trop.F90449ukca_chem_strat.F90450! Aerosol chemistry: there are no gas phase products, the 'NULLx' productsukca_chem_strat.F90451! identify the reactions in asad_heteroukca_chem_tropisop.F90452TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ &ukca_chemco.F90453!HS03+H202(aq)ukca_chemistry_ctl.F90455', 0.000, 0.000, 0.000), 0.000), 0.000), 0.000), 0.000), &	ukca_chem1_dat.F90		
ukca_chem_defs_mod.F90448ukca_chem_arq.F90449ukca_chem_std_trop.F90450ukca_chem_strat.F90450ukca_chem_strat.F90451ukca_chem_strattrop.F90451ukca_chem_tropisop.F90452ukca_chemco.F90453ukca_chemco_raq.F90454rath_t('S02','H202ukca_chemistry_ctl.F90455ukca_chemistry_ctl.F90 <t< td=""><td>ukca_chem_aer.F90</td><td></td><td></td></t<>	ukca_chem_aer.F90		
ukca_chem_raq.F90449ukca_chem_strat.F90450! Aerosol chemistry: there are no gas phase products, the 'NULLx' productsukca_chem_strat.F90451! identify the reactions in asad_heteroukca_chem_tropisop.F90452TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ &ukca_chemco.F90453!HS03+H202(aq)ukca_chemistry_ctl.F90455' , 0.000, 0.000, 0.000, 0.000), .ukca_chemistry_ctl.F90455' , 0.000, 0.000, 0.000), 0.000), .	ukca_chem_defs_mod.F90	12	
ukca_chem_std_trop.F90450! Aerosol chemistry: there are no gas phase products, the 'NULLx' productsukca_chem_strattrop.F90450! Aerosol chemistry: there are no gas phase products, the 'NULLx' productsukca_chem_strattrop.F90451! identify the reactions in asad_heteroukca_chemco.F90452TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ &ukca_chemco_raq.F90454rath_t('S02ukca_chemistry_ctl.F90455' ,0.000, 0.000, 0.000, 0.000),	ukca_chem_raq.F90		
ukca_chem_strattrop.F90 451 ! identify the reactions in asad_hetero ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco.F90 453 !HS03+H202(aq) ukca_chemistry_ctl.F90 454 rath_t('S02 ','H202 ','NULL0 ',' ', & ukca_chemistry_ctl.F90 455 ' ',0.000, 0.000, 0.000), 0.000), 0.000), 0.000), 0.000), 0.000), 0.000), 0.000) &			
ukca_chem_tropisop.F90 452 TYPE(RATH_T) :: rath_defs_strattrop_aer(1:nhet_st_aer)=(/ & ukca_chemco.F90 453 !HS03+H202(aq) ukca_chemco_raq.F90 454 rath_t('S02 ', 'H202 ', 'NULL0 ', ' ', & ukca_chemistry_ctl.F90 455 ' ', 0.000, 0.000, 0.000), 0.000), 0.000), & & &			
ukca_chemco_F90 453 1HS03+H202(aq) ukca_chemco_raq.F90 454 rath_t('S02 ','H202 ','NULL0 ',' ', & ukca_chemistry_ctl.F90 455 ' ',0.000, 0.000, 0.000), 0.000), 0.000), & & &			
ukca_chemico_raq.F90 454 rath_t('S02 ','H202 ','NULL0 ',' ', & ukca_chemistry_ctl.F90 455 ' ',0.000, 0.000, 0.000, 0.000), & &			
ukca_chemistry_ctl.F90 455 ', 0.000, 0.000, 0.000, 0.000), &	_		
ukca_cloudproc.F90 456 !HS03+03(aq)			
ukca_coag_coff_v.F90 457 rath t('S02 '.'03 '.'NULL1 '.' '.' '. &		456 !HS03+03(aq)	
	ukca_coagwithnucl.F90	458 '. 0.000. 0.000. 0.000). &	

UKCA/ukca_hetero_mod.F90

ukca_extract_d1_integer_data2d.	⊲ ⊳ ukca h	hetero_mod.F90	
ukca_extract_d1_logical_data2d.		-	756.0
ukca_fastj.F90	110	INTEGER, SAVE :: N_NOCL_NCL=0	
ukca_fastjx.F90	112	LOGICAL, SAVE :: first = .TRUE.	-lin
ukca_fdiss.F90	112	EUGICAE, SAVE THISETROE.	100
ukca_feedback_mod.F90		REAL is an(theta field cize)	
ukca_fixeds.F90	114	REAL :: zp(theta_field_size)	1.0000
ukca_fixedsb.F90	115	REAL :: zt(theta_field_size)	1
ukca_flupj.F90	116	REAL :: zhno3(theta_field_size)	2
ukca_fracdiss.F90	117	REAL :: zh2o(theta_field_size)	
ukca_hetero_mod.F90	118	REAL :: zhcl(theta_field_size)	<u></u>
ukca_impc_scav.F90	119	REAL :: zclono2(theta_field_size)	
ukca_inddep.F90	120	REAL :: zn2o5(theta_field_size)	- 100 more
ukca_ingridg.F90	121	REAL :: zhocl(theta_field_size)	100
ukca_iniasad.F90	122	REAL :: psc1(theta_field_size)	2 tot
ukca_init.F90	123	REAL :: psc2(theta_field_size)	
ukca_interp.F90	124	REAL :: psc3(theta_field_size)	and the second s
ukca_inwdep.F90	125	REAL :: psc4(theta_field_size)	101100 101100 101100 10100
ukca_light.F90	126	REAL :: psc5(theta_field_size)	100
ukca_light_ctl.F90	127	REAL :: hk(theta_field_size,5)	To T
ukca_main1-ukca_main0.F90	128		International Statement
ukca_main1-ukca_main1.F90	129	<pre>INTEGER(KIND=jpim), PARAMETER :: zhook_in = 0</pre>	-Rame-
ukca_mode_check_artefacts_moc	130	<pre>INTEGER(KIND=jpim), PARAMETER :: zhook_out = 1</pre>	
ukca_mode_ems_mod.F90	131	REAL(KIND=jprb) :: zhook_handle	-gran.
ukca_mode_ems_um_mod.F90	132		The second secon
ukca_mode_setup.F90	133 🔻 !		Zenepurc
ukca_nstypes.F90	134		1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 - 1000 -
ukca_option_mod.F90 ukca_phot2d.F90	135	<pre>IF (lhook) CALL dr_hook('UKCA_HETER0_MOD:UKCA_HETER0',zhook_in,zhook_handle)</pre>	10100
ukca_photol.F90	136 🔻	IF (first) THEN	10eta
ukca_prim_car.F90	137 🔻	DO js = 1, jpctr	
ukca_prim_car.r90 ukca_prim_ss.F90	138 🔻	SELECT CASE (advt(js))	1 March March
ukca_prim_su.F90	139	CASE ('H20 ', 'H20S ')	
ukca_radaer_band_average.F90	140	ih2o = js	17
ukca_radaer_compute_aod.F90	141	CASE ('HONO2 ')	20.75.7
ukca_radaer_get.F90	142	ihno3 = js	- C 10

UKCA/ukca_chem_hetero_mod.F90

uken autract dl integer datald	~/Dropbox/source/UM/vn8.4_vanilla/src/atmosphere/UKCA/ukca_hetero_mod.F90 — UKCA	
ukca_extract_d1_integer_data2d. ukca_extract_d1_logical_data2d.	d b ukca_hetero_mod.F90	
ukca_fastj.F90	630 END IF	III=
ukca_fastjx.F90	631 !	
ukca_fdiss.F90	632 END IF	10
ukca_feedback_mod.F90	633 1	- Elinear
ukca_fixeds.F90	634 !	1.0.8
ukca_fixedsb.F90	635 ! 4. AEROSOL REACTIONS	
ukca_flupj.F90	636 !	
ukca_fracdiss.F90	637 !	10.
ukca_hetero_mod.F90	638 ! If required, include the reactions on the sulphate aerosols.	1000-000
ukca_impc_scav.F90	639 IF (LPSA) THEN	1010
ukca_inddep.F90	640 T 1	100000
ukca_ingridg.F90	641 CALL UKCA_EQCOMP(T,TH20,KSTART,KEND,KCHMLEV,LPHOCL, &	
ukca_iniasad.F90	642 GAM3B,HSHCL,HHOCL)	WEID IN
ukca_init.F90	643 T 1	2
ukca_interp.F90		1000 - 1000 1000 - 1000 1000 - 1000 1000 - 1000 1000 - 1000
ukca_inwdep.F90	644 AKPSC2(kstart:kend) = AKPSC2(kstart:kend) + &	100 miles 100 miles 100 miles
ukca_light.F90	645 CCNIT(kstart:kend)*100.0*SASA(kstart:kend)*GAM3B(kstart:kend)	100 Per 100 PE
ukca_light_ctl.F90	646 AKPSC3(kstart:kend) = AKPSC3(kstart:kend) + &	100 cm 100 1744 -
ukca_main1-ukca_main0.F90	647 CN205(kstart:kend)*100.0*SASA(kstart:kend)*GAM3C	1000
ukca_main1-ukca_main1.F90	648 !	Terre Terre
ukca_mode_check_artefacts_moc	649 ▼ ! If required, include HOCl + HCl -> Cl2 + H2O	
ukca_mode_ems_mod.F90	650 IF (LPHOCL)THEN	The second se
ukca_mode_ems_um_mod.F90	651 DO JL = KSTART , KEND	in an and a second s
ukca_mode_setup.F90	652 !	
ukca_nstypes.F90	653 ! Estimate specific volume from surface area	T AND A
ukca_option_mod.F90	654 VOL = SASA(JL)*RADSA/3.0	1000
ukca_phot2d.F90	655 !	PHE.
ukca_photol.F90	656 7 ! Add aerosol rate, converted to pseudo first order	The second se
ukca_prim_car.F90	657 ORDER2=1.E6*CPK1*VOL*AVOGAD*HSHCL(JL)*HHOCL(JL)*	
ukca_prim_ss.F90	658 (BOLTZ*T(JL))**2.0	
ukca_prim_su.F90	659 AKPSC5(JL) = AKPSC5(JL) + ORDER2*THCL(JL)	100
ukca_radaer_band_average.F90	660 END DO	THE REPORT OF TH

UKCA/ukca_chem_hetero_mod.F90

ukca_extract_01_integer_0ata20.	↓ ukca_hetero_mod.F90		=
ukca_extract_d1_logical_data2d.		1 1	
ukca_fastj.F90	631 !		le-u
ukca_fastjx.F90	632 END IF	10	127 1 km
ukca_fdiss.F90	633 !		
ukca_feedback_mod.F90	634 !		
ukca_fixeds.F90			
ukca_fixedsb.F90			
ukca_flupj.F90	636 !		Ł
ukca_fracdiss.F90	637 !		
ukca_hetero_mod.F90	638 ! If required, include the reactions on the sulphate aerosols.		
ukca_impc_scav.F90	639 IF (LPSA) THEN		
ukca_inddep.F90	640 7 !		10001
ukca_ingridg.F90	641 CALL UKCA_EQCOMP(T,TH20,KSTART,KEND,KCHMLEV,LPHOCL,	&	in a second s
ukca_iniasad.F90	642 GAM3B,HSHCL,HHOCL)	1	
ukca_init.F90	643 🔻 !	3	Concession in the local division of the loca
ukca_interp.F90	644 AKPSC2(kstart:kend) = AKPSC2(kstart:kend) +	&	and the second
ukca_inwdep.F90	645 CCNIT(kstart:kend)*100.0*SASA(kstart:kend)*GAM3B(kstart:kend)	= (b	
ukca_light.F90	646 AKPSC3(kstart:kend) = AKPSC3(kstart:kend) +	&	
ukca_light_ctl.F90	647 CN205(kstart:kend)*100.0*SASA(kstart:kend)*GAM3C		No.
ukca_main1-ukca_main0.F90	648 !	1	a Sil'ilan
ukca_main1-ukca_main1.F90	649 ▼ ! If required, include HOCl + HCl -> Cl2 + H2O		Sec 1
ukca_mode_check_artefacts_moc	650 IF (LPHOCL)THEN		
ukca_mode_ems_mod.F90	651 DO JL = KSTART , KEND		
ukca_mode_ems_um_mod.F90	652 !		
ukca_mode_setup.F90	653 ! Estimate specific volume from surface area		-550c
ukca_nstypes.F90	654 VOL = SASA(JL)*RADSA/3.0		I BIRGHTA
ukca_option_mod.F90	655 I		10. m
ukca_phot2d.F90	656 7 ! Add aerosol rate, converted to pseudo first order		L.L.
ukca_photol.F90		8	
ukca_prim_car.F90		×	
ukca_prim_ss.F90	658 (BOLTZ*T(JL))**2.0		-
ukca_prim_su.F90	659 AKPSC5(JL) = AKPSC5(JL) + ORDER2*THCL(JL)		E.
ukca_radaer_band_average.F90	660 END DO	1	annes annes

The MODE aerosol chemistry - slightly different

UKCA/ukca_chem_strattrop.F90

ukca_ciouupioc.i 50	466								
ukca_coag_coff_v.F90	467	! Tropospheric	heterogenous	reactions					
ukca_coagwithnucl.F90	468			trattrop_trophe	t(1:nhet s	t toht)=(/		&	
ukca_cond_coff_v.F90	469	! Heterogenous		er a c c r op_er oprio		<u></u>		~	
ukca_conden.F90	470	rath_t('N205	1,1	', 'HONO2	','	1,1	۰,	&	
ukca_constants.F90	471	· ·		0.000, 0.000),				&	
ukca_cspecies.F90	472	! Heterogenous		,,				-	
ukca_d1_defs.F90	473	rath_t('HO2	','	','H202	1,1	1,1	۰,	&	
ukca_dcoff_par_av_k.F90	474	· ·	0.500, 0.000,	0.000, 0.000)	-		-	&	
ukca_ddcalc.F90	475	/)	,	,,				-	
ukca_ddepaer.F90	476	/ <u>/</u>							
ukca_ddepaer_incl_sedi.F90	477								

UKCA/ukca_main1-ukca_main1.F90

OPEN FILES	$\triangleleft \triangleright$	ukca_chem_strattrop.F90	Find Results	ukca_aer	o_ctl.F90	ukca_main1-ukca_main1.F90	ukca_e
Find Results				1	-		
ukca_aero_ctl.F90		/ DEPENDS ON: ukca_aero_ctl	ath if day and an if have				
ukca_main1-ukca_main1.F90	2113	I_minute - INT(tim	nth, i_day_number, i_hour,	2			
	2115	REAL(interval)*tim		e.			
ukca_chemistry_ctl.F90	2116	model_levels, rows		8			
FOLDERS	2117	wet_levels,		84			
🔻 🚔 UKCA	2118	global_row_length,	global_rows,	8			
▶ m photolib	2119	n_chem_tracers+n_a	ero_tracers,	8.			
asad_bedriv.F90	2120	n_mode_tracers,		8.			
	2121	het_dimn, nhet_std	_trop,	84			
asad_bimol.F90	2122	area,		8			
asad_cdrive.F90	2123		th,l:rows)/two_omega,	ě.			
asad_chem_flux_diags.F90	2124 2125	true_longitude,	ude(1:row_length,1:rows),	2			
asad_cinit.F90	2125		ow_length,1:rows,1:model_levels),	2			
	2127		ow_length,1:rows,:),	2			
asad_diffun.F90	2128		ows,1:model_levels),	8			
asad_emissn.F90	2129		ow_length,1:rows,:),	8.			
asad_findreaction.F90	2130	rel_humid_clr (1:r	ow_length,1:rows,:),	8			
asad_flux_dat.F90	2131	p_layer_boundaries	(1:row_length,1:rows,0:model_levels),	8.			
	2132	all_tracers(1:row_	<pre>length,1:rows,1:model_levels,</pre>	8.			
asad_ftoy.F90	2133	1:n_chem_trac	ers+n_aero_tracers),	8			
asad_fuljac.F90	2134		<pre>length,1:rows,1:model_levels,</pre>	8.			
asad_fyfixr.F90	2135		s+n_aero_tracers+1:	8			
asad_fyinit.F90	2136		s+n_aero_tracers+	8			
asad_fyself.F90	2137 2138	n_mode_tracer		ĉ			
	2130	Tstar(1:row_length seaice_frac(1:row_		ž			
asad_hetero.F90	2140	Rough_length(1:row		í.			
asad_impact.F90	2141	u_s,		84			
asad_inemit.F90	2142	U_scalar_10m,		8.			
asad_inhet.F90	2143		<pre>ngth,1:rows,1:model_levels),</pre>	8.			
	2144	conv_rain3d(1:row_	<pre>length,1:rows,1:model_levels),</pre>	8.			
asad_inicnt.F90	2145		<pre>ngth,1:rows,1:model_levels),</pre>	8.			
asad_inijac.F90	2146		<pre>length,1:rows,1:model_levels),</pre>	8.			
asad_inimpct.F90	2147		<pre>gth,1:rows,1:wet_levels),</pre>	84			
asad_inix.F90	2148		<pre>ngth,1:rows,1:wet_levels),</pre>	8			
_	2149		th,l:rows,l:wet_levels),	ě.			
asad_inphot.F90	2150 2151	land_fraction,	<pre>th,1:rows,1:wet_levels),</pre>	e e			
asad_inrats.F90	2152	theta_field_size*m	odel levels,	8			
asad_jac.F90	2153	delso2_wet_h2o2,	,	8.			
asad_mod.F90	2154	delso2_wet_o3,		8			
asad_posthet.F90	2155	delh2so4_chem,		8.			
asad_pris.F90	2156	mode_diags,		8.			
	2157	het_rates,		84			
acad cotstaady EQO	2150	cloud fracilitrow h	anoth licour limodal louals)				

UKCA/ukca_main1-ukca_main1.F90

UPEN FILES	$\triangleleft \triangleright$	ukca_chem_strattrop.F90	Find Results	ukca_aero_ctl.F90	ukca_main1-ukca_main1.F90	ukca_chemistry_ctl.F90
Find Results	2156	mode_diags,				Shere
ukca_aero_ctl.F90	2157	het_rates,		6		10000
ukca_main1-ukca_main1.F90	2158		<pre>length,1:rows,1:model_levels</pre>	i), &		Der Sternen Sterne
ukca_chemistry_ctl.F90	2159	cloud_liq_frac(1:	row_length,1:rows,1:model_le	rvels), &		
	2160	cloud_liq_water(1	:row_length,1:rows,1:model_1	levels), &		
DLDERS	2161	offx, offy,		a.		10000
🚔 UKCA	2162	z_half_alllevs, d	elta_r,	8		175.0
photolib	2163 2164	volume,mass,zbl, uph2so4inaer,				
asad_bedriv.F90	2165	wetox_in_aer,				We was
asad_bimol.F90	2166	chem_diags(:,:,:,	icd_cdnc),	6		-1050cc -1050cc
	2167	chem_diags(:,:,:,				-806865
asad_cdrive.F90	2168)				
asad_chem_flux_diags.F90	2169 🔻			ny l		1200000
asad_cinit.F90	2170 🔻					10 Million
asad_diffun.F90	2171 🔻					C.C.S. *
asad_emissn.F90	2172 2173		<pre>length,1:rows,:,10) = es(:,1),(/row_length,rows,module)</pre>	s del louels/l)		"Planar
asad_findreaction.F90	2174		length,1:rows,:,11) =	&		"Else-
	2175		es(:,2),(/row_length,rows,mo	del_levels/))		
asad_flux_dat.F90	2176 🔻					68.88
asad_ftoy.F90	2177	cmessage='Not end	ugh space for Heterogenous F	lates'		100
asad_fuljac.F90	2178	icode = 1				
asad_fyfixr.F90	2179		A_MAIN1',icode,cmessage)			10
asad_fyinit.F90	2180 2181		em_diags >= 11 a_trophet			Energy Witten
asad_fyself.F90	2182	eno ar	a_ ci opini c			30 of ce
	2183	I DEPENDS ON: timer				Par
asad_hetero.F90	2184	IF (ltimer) CALL TIMER	('UKCA AEROSOL MODEL ',6)			
asad_impact.F90	2185					Same -
asad_inemit.F90	2186	I Call activation scheme if sw				Distant.
asad_inhet.F90	2187	IF(L_ukca_arg_act) THE	N			1
asad_inicnt.F90	2188	I DEPENDS ON: ukca_activate				COMPRESS OF
asad_inijac.F90	2189 7					
	2191		, model_levels, wet_levels,	4		THE TANK
asad_inimpct.F90	2192	bl_levels,		4		E COM
asad_inix.F90	2193	theta_field_size		8		TODE CONTRACTOR
asad_inphot.F90	2194	n_mode_tracers,		A		Librar
asad_inrats.F90	2195	n_mode_diags, n	_chem_diags,			10/1/00
asad_jac.F90	2196	tr_index,	- leasth larger bandel la	1. E		
	2197 V 2198		w_length,l:rows,l:model_leve n_aero_tracers+l:	×, ×		1000
asad_mod.F90	2198		n_aero_tracers+n_mode_tracer	(5), 8		
asad_posthet.F90	2200	mode_diags, chem		4		1
asad_pris.F90	2201		:row_length,1:rows,1:model_1	levels), &		Dim

UKCA/ukca_main1-ukca_main1.F90

ukca_ch4_stratloss.F90	< ⊳ F	Find Results	ukca_aero_ctl.F90	ukca_main1-ukca_main1.F90	ukca_chemistry_ctl.F90	
	1000 -	L DEDENDE ONA scheme als sel	ster et]			10
ukca_check_md_nd.F90	1969 🗸	DEPENDS ON: ukca_chemi	<pre>STRY_CTL(I_month, I_day_number, I_hour,</pre>			"Boosrun
ukca_chem1_dat.F90	1971		INT(timestep)/60,	2		No.
ukca_chem_aer.F90	1972		al)*timestep,	8		
ukca_chem_defs_mod.F90	1973		ers+n_aero_tracers, n_chem_diags,	8		10 Delmont
ukca_chem_raq.F90	1974	n_BE_fluxdi	ags,	8		
ukca_chem_std_trop.F90	1975	f3_at_u(1:r	ow_length,1:rows)/two_omega,	8		
	1976		a_latitude(1:row_length,1:rows),	6		
ukca_chem_strat.F90	1977 1978	true_longit	ude, els(1:row_length,1:rows,1:model_levels)	a		
ukca_chem_strattrop.F90	1979		<pre>w_length,1:rows,1:model_levels),</pre>	, <u>,</u>		Electronic States of State
ukca_chem_tropisop.F90	1980		w_length,1:rows,1:model_levels),	8		PLAN AND A
ukca_chemco.F90	1981		ength,1:rows,1:model_levels),	6		- Paller
ukca_chemco_raq.F90	1982	qcl(1:row_l	ength, 1:rows,1:model_levels),	6		8 ²²
ukca_chemistry_ctl.F90	1983		<pre>rac(1:row_length,1:rows,1:model_levels)</pre>			2988
	1984		ndaries(1:row_length,1:rows,0:model_lev	els), &		2 Million
ukca_cloudproc.F90	1985		els(1:row_length, 1:rows, :),	<u>.</u>		100000
ukca_coag_coff_v.F90	1986 1987	<pre>z_top_of_mo cos_zenith_</pre>		ě.		100005
ukca_coagwithnucl.F90	1988		<pre>(1:row_length,1:rows,1:model_levels,</pre>	2		
ukca_cond_coff_v.F90	1989		1:n_chem_tracers+n_aero_tracers),	6		Sector Se
ukca_conden.F90	1990	chen_diags(1:row_length,1:rows,:,:),	6		
ukca_constants.F90	1991	BE_fluxdiag	s(l:row_length,l:rows,:,:),	8		Comment.
	1992	Tstar,		6		Contraction of the second s
ukca_cspecies.F90	1993	Thick_bl_le		ŝ.		and the second se
ukca_d1_defs.F90	1994 1995	Rough_lengt u_s,	n,	а 8		
ukca_dcoff_par_av_k.F90	1996	ls_ppn3d, c	onv_ppn3d.	2		
ukca_ddcalc.F90	1997		1:row_length, 1:rows, :),	6		
ukca_ddepaer.F90	1998	dj(:,:,:,:)	,	8		177.00. 1015.01
ukca_ddepaer_incl_sedi.F90	1999	volume(:,:,	:),	6		11
	2000	mass(:,:,:)		8		No. 1920.
ukca_ddepctl.F90	2001 🔻		w dry dep scheme			- constant
ukca_ddeprt.F90	2002		, land_index, ile_index, tile_frac,	6 8		- 10000 cm. - 10000 cm. - 10000 cm. - 10000 cm.
ukca_deriv.F90	2004		f, seaice_frac, stcon,	2		1000 Contraction of the local data and the local da
ukca_deriv_aero.F90	2005		moisture(:,1), fland,	6		10000000
ukca_deriv_raq.F90	2006	laift_lp, c		6		- Martin
	2007		tstar_tile, canwctile_lp,	6		Contraction of the local distance of the loc
ukca_dissoc.F90	2008	pv_on_theta		8		"Planear
ukca_diurnal_isop_ems.F90	2009		_length,l:rows,l:model_levels),			Picture Title and Title and Ti
ukca_drydep.F90	2010	um_ozone3d,		2		Silena Silena
ukca_emission_ctl.F90	2011 2012	uph2so4inae delso2_wet_		2		17. C.
ukca_extract_d1_data1d.F90	2013	delso2_wet_		6		parts.
ukca_extract_d1_data2d.F90	2014	delh2so4_ch				Contractor in

ukca_ch4_stratloss.F90		uxca_aeio_cu.r50	ukca_chemistry_cu.r.50	
ukca_check_md_nd.F90	21 - 1 1 1		d day anabaa d baya d	No. optimise With Annual Statement
ukca_chem1_dat.F90	31 - 32	SUBROUTINE UKCA_CHEMISTRY_CTL(i_month, i_minute, secs_per_step		E
ukca_chem_aer.F90	33	ntracers,	ν, α κ	
ukca_chem_defs_mod.F90	34	ndiags,		Sta.
ukca_chem_raq.F90	35	nfluxdiags,		
ukca_chem_std_trop.F90	36	sinlat,	6	Sector Se
ukca_chem_strat.F90	37	coslat,	ě.	
ukca_chem_strattrop.F90	38	true_longitude,	8.	III."
	39	pres, temp, q,	8	100 11 5
ukca_chem_tropisop.F90	40	qcf, qcl, rh,	8	
ukca_chemco.F90	41	p_layer_boundaries,	84	ITHERE
ukca_chemco_raq.F90	42	<pre>r_theta_levels,</pre>	8	
ukca_chemistry_ctl.F90	43	<pre>z_top_of_model,</pre>	8	1.
ukca_cloudproc.F90	44	cos_zenith_angle,	8	111 (2822)
ukca_coag_coff_v.F90	45	tracer,	8	
ukca_coagwithnucl.F90	46 47	user_diags,	6	1 1 52:02
ukca_cond_coff_v.F90	48	mflux_diags, t_surf, dzl, z0m, u_s,	°,	**************************************
ukca_conden.F90	49	drain, crain,	ž	"Illusion or a second
ukca_constants.F90	50	cloud_frac,		I I I I
ukca_cspecies.F90	51	fastj_dj,	6	k diaman
ukca_d1_defs.F90	52	volume, mass,	6	
ukca_dcoff_par_av_k.F90	53	land_points, land_index	د, ه	10
ukca_ddcalc.F90	54	tile_pts, tile_index, t	tile_frac, &	1158 Moor 1182 Mar 1189
ukca_ddepaer.F90	55	zbl, surf_hf, seaice_fr	rac, stcon, &	
ukca_ddepaer_incl_sedi.F90	56	soilmc_lp, fland, laift		
ukca_ddepctl.F90	57	z0tile_lp, t0tile_lp, d	canwctile_lp, &	
ukca_ddeprt.F90	58	pv_at_theta,	8	
ukca_deriv.F90	59	theta,	8	E II II- "E ALE AND
ukca_deriv_aero.F90	60 61	um_ozone3d, uph2so4inaer,	۵	Shift opport
ukca_deriv_raq.F90	62	delso2_wet_h2o2,	e e e e e e e e e e e e e e e e e e e	in and a set of the se
ukca_dissoc.F90	63	delso2_wet_03,	Ĩ.	154585
ukca_diurnal_isop_ems.F90	64	delh2so4_chem,	a a	
ukca_drydep.F90	65	delso2_drydep,	6	20 State Street
ukca_emission_ctl.F90	66	delso2_wetdep,	8.	Maria and C
ukca_extract_d1_data1d.F90	67	so4_sa	&	1950-00
ukca_extract_d1_data2d.F90	6.8	<u>)</u>		
ukca_extract_01_0ata20.F90	63			

ukca_ch4_stratloss.F90	⊲ ⊳ Find Re	sults	ukca_aero_ctl.F90	ukca_chemistry_ctl.F90		Sharing Screenshot
ukca_check_md_nd.F90	243	REAL :: zclw	(theta_field_size)	! 1-D cloud liqui	d water	A link to your screenshot has be clipboard (click to view).
ukca_chem1_dat.F90	244		oud(theta_field_size)	! 1-D cloud fract		
ukca_chem_aer.F90	245		(theta_field_size,jpct			
ukca_chem_defs_mod.F90	246		heta_field_size)	! 1-D water vapou	-	
ukca_chem_raq.F90	247		da(rows, ntphot, jppj)			
ukca_chem_std_trop.F90	248		(row_length, rows, jpp			
ukca_chem_strat.F90	249	-	<pre>ld(theta_field_size,jp</pre>			
ukca_chem_strattrop.F90	250		(row_length, rows)	! local time		
ukca_chem_tropisop.F90	251		en(row_length, rows)	! local daylength	1	
ukca_chemco.F90	252	-	our_ang(row_length, ro			
ukca_chemco_raq.F90	253		at(row_length, rows)	! tangens of lati		
ukca_chemistry_ctl.F90	254		rt(row_length, rows, j	U U	dry dep rate	
ukca_cloudproc.F90	255	-	rt2(theta_field_size,		dry dep rate	
ukca_coag_coff_v.F90	256		rt(row_length, rows, m		wet dep rate	
ukca_coagwithnucl.F90	257		rt2(theta_field_size,		wet dep rat	
ukca_cond_coff_v.F90	258		rt3(theta_field_size,			
ukca_conden.F90	259		iss2(theta_field_size,	- , , , , ,	dissolved fr	action
ukca_constants.F90	260		iss(row_length, rows,		peq+1)	
ukca_cspecies.F90	261		et(theta_field_size,2)		erog rates fo	r trop chem
ukca_d1_defs.F90	262		h(row_length, rows, mo		sociation con	
ukca_dcoff_par_av_k.F90	263		h2(theta_field_size)		sociation con	st
ukca_ddcalc.F90	264	REAL :: ozon	ecol(row_length, rows,	<pre>model_levels) ! for</pre>	strat chem	
ukca_ddepaer.F90	265	REAL :: BE_t	nd(theta_field_size)	! tot	al no density	
ukca_ddepaer_incl_sedi.F90	266	REAL :: BE_h	2o(theta_field_size)	! wat	er vapour con	cn
ukca_ddepctl.F90	267	REAL :: BE_O	2(theta_field_size)	! oxy	gen concn	
ukca_ddeprt.F90	268	REAL :: BE_v	ol(theta_field_size)	l gri	dbox volume	
ukca_deriv.F90	269	REAL :: BE_w	etrt(theta_field_size,	jpspec) ! wet	dep rates (s	-1)
ukca_deriv_aero.F90	270	REAL :: BE_d	ryrt(theta_field_size,	jpspec) ! dry	dep rates (s	-1)
ukca_deriv_raq.F90	271	REAL :: BE_d	eprt(theta_field_size,	jpspec) ! dep	rates (s-1)	
ukca_dissoc.F90	272	REAL :: BE_f	rdiss(theta_field_size	<pre>,jpspec,jpeq+1) ! dis</pre>	solved fraction	on
ukca_diurnal_isop_ems.F90	273		(theta_field_size,jps			
ukca_drydep.F90	274	REAL :: stra	t_ch4loss(theta_field_	size,model_levels) !	for strat ch4	loss
ukca_emission_ctl.F90	275		s(theta_field_size,5)		rate coeffs	

		~/Diohpox/s	SUULCE/UNI/VIIO.4_ValIIIIa/SIC/a	annosphere/OKCA/ukca_chemistry_c	U.F90 - UKCA
ukca_ch4_stratloss.F90	$\triangleleft \triangleright$	Find Results	ukca_aero_ctl.F90	ukca_chemistry_ctl.F90	
ukca_check_md_nd.F90			rru		())
ukca_chem1_dat.F90	661		I(:, I) = RESHAPE(Zprt	<pre>(:,:,l),(/theta_field_size</pre>	())
ukca_chem_aer.F90	662				
ukca_chem_defs_mod.F90	663 664		D routines to do cha	mietry integration	
ukca_chem_raq.F90			ND routines to do cher	the dynamical timestep fo	
ukca_chem_std_trop.F90	665			step > 20 min, use half an	
ukca_chem_strat.F90	667		of dynamical timeste		10
ukca_chem_strattrop.F90	668		or dynamical timeste	p for chemistry.	
ukca_chem_tropisop.F90			(Lukes tree OP L	ukes sercher OP	0
ukca_chemco.F90	669		.(L_ukca_trop .OR. L	_ukca_aerchem .uk. ! Not	- P_E
ukca_chemco_raq.F90	671		L_ukca_raq)) THEN	: NOT	D-C
ukca_chemistry_ctl.F90	672		eric flag indicator a	and SOA surface area	
ukca_cloudproc.F90	673		<u> </u>	rates from previous time	stop
ukca_coag_coff_v.F90	674		ikca_trophet) THEN	races from previous crime	step
ukca_coagwithnucl.F90	675		net(:,1) = RESHAPE(use	ar diage(· · k 10)	&
ukca_cond_coff_v.F90	676			theta_field_size/))	! N205
ukca_conden.F90	677		net(:,2) = RESHAPE(use		. N205
ukca_constants.F90	678			theta_field_size/))	1 H02+H02
ukca_cspecies.F90	679			checa_fieta_size///	1 102 1102
ukca_d1_defs.F90	680		lag(:) = (NOT RESH	APE(L_troposphere(:,:,k),	8.
ukca_dcoff_par_av_k.F90	681			<pre>(/theta_field_size/)))</pre>	Ck.
ukca_ddcalc.F90	682			<pre>,k),(/theta_field_size/))</pre>	
ukca_ddepaer.F90	683		- 1201712(304_30(1))	, , , , , , , , , , , , , , , , , , ,	
ukca_ddepaer_incl_sedi.F90	684		thod == 3) THEN		
ukca_ddepctl.F90	685		,	: 1 hour. Note that in thi	S C250
ukca_ddeprt.F90	686			every 2nd/3rd dynamical ti	
ukca_deriv.F90	687	_	- ,	and dtime should equal 1 h	
ukca_deriv_aero.F90	688			Raphson contains automatic	
ukca_deriv_raq.F90	689		Conter Benee Hencoll	aprison concerns acconacte	00000000
ukca_dissoc.F90	690		is the *CHEMISTRY* +	imestep and not the model	timesten.
ukca_diurnal_isop_ems.F90	691			e INTERVAL=3600/INT(TIMEST	
ukca_drydep.F90	692		en chemistry is called		
ukca_emission_ctl.F90	693		· ·	2 changed 2010/02/08 20	1.40

ukca_ch4_stratloss.F90			ukca_aero_ctl.F90	ukca_chemistry_ctl.F90	•
ukca_check_md_nd.F90	701 -	ELSE			•
ukca_chem1_dat.F90	702		= 0.5*dtime		
ukca_chem_aer.F90	703		eps = 2		
ukca_chem_defs_mod.F90	704	END IF			
ukca_chem_raq.F90	705	END IF			
ukca_chem_std_trop.F90	706				
ukca_chem_strat.F90	707				
ukca_chem_strattrop.F90	708	IF (uph2	so4inaer == 1) THEN		
ukca_chem_tropisop.F90			dated in MODE, so st	tore old value here	
ukca_chemco.F90	710		(:) = y(:,nn_h2so4)		
ukca_chemco_raq.F90	711	END IF	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
ukca_chemistry_ctl.F90	712				
ukca_cloudproc.F90		ENDS ON: asad	cdrive		
ukca_coag_coff_v.F90	714 🔻		D_CDRIVE(cdot, zftr,	. zp. zt. zg.	8.
ukca_coagwithnucl.F90	715			oud_frac(:,:,k),(/n_pnts/)),	8.
ukca_cond_coff_v.F90	716			l(:,:,k),(/n_pnts/)),	8.
ukca_conden.F90	717			zwetrt3, rc_het,	&
ukca_constants.F90	718			pnts, stratflag)	
ukca_cspecies.F90	719		, , , , , , , , , , , , , , , , , , , ,	,	
ukca_d1_defs.F90	720	IF (L uk	ca_het_psc) THEN		
ukca_dcoff_par_av_k.F90			, ,	3-D array for PSC sedimentation.	
ukca_ddcalc.F90			is NAT in number de		
ukca_ddepaer.F90				eld_size) > 0.)) THEN	
ukca_ddepaer_incl_sedi.F90	724			<pre>PE(sphno3(:)/tnd(:),</pre>	&
ukca_ddepctl.F90	725			row_length,rows/))*c_hono2	
ukca_ddeprt.F90	726	ELSE			
ukca_deriv.F90	727		3_3d(:,:,k) = 0.		
ukca_deriv_aero.F90	728	END IF	, , .		
ukca_deriv_raq.F90	729	END IF			
ukca_dissoc.F90	730				
ukca_diurnal_isop_ems.F90	731	! CODV O	ver O(1D) into chem	diags	
ukca_drydep.F90	732 🔻	IF (LVMR			
ukca_emission_ctl.F90	733		diags(1:row_length,	1:rows.k.1) = k	

UKCA/asad_cdrive.F90

sad_bedriv.F90	< ► Find Results		ukca_aero	_ctl.F90	ukca_chemistry	y_ctl.F90	asad_cdrive	e.F90
asad_bimol.F90	0.0	USE werkeek	0111	Theoly dis book			,	
asad_cdrive.F90	96 97	, ,		lhook, dr_hook				
asad_chem_flux_diags.F90	98	USE ereport_		LY : ereport				
asad_cinit.F90	99	USE UM_ParVa USE Control_						
asad_diffun.F90	100	IMPLICIT NON	_	65				
asad_emissn.F90	101	IMPLICIT NON	E					
asad_findreaction.F90		le "typsize.h"						
asad_flux_dat.F90	102 #110000	e cypsize.n.						
asad_ftoy.F90		outine interfa	Ce					
asad_fuljac.F90	105			:: n_points		! No of po	ints	
asad_fyfixr.F90	106	INTEGER, INT				! Model le		
asad_fyinit.F90	107	20020200 200						
asad_fyself.F90	108	REAL, INTENT	(IN) ::	prt(n_points,	ippi)	! Photolys	is rates	
asad_hetero.F90	109	,		dryrt(n_point		! Dry dep		
asad_impact.F90	110	-		wetrt(n_point				rates
asad_inemit.F90	111			rc_het(n_poin		! Hetero.		
asad_inhet.F90	112			pp(n_points)	,-,	! Pressure	-	
asad_inicnt.F90	113			pt(n_points)		! Temperat		
asad_inijac.F90	114	-		pq(n_points)		! Water va		
asad_inimpct.F90	115	-		cld_f(n_point	s)	! Cloud fr		
asad_inix.F90	116			cld_l(n_point	-	! Cloud li	quid wate	r (kg/kg)
asad_inphot.F90	117	-		:: stratflag(-	! Strat in	-	
asad_inrats.F90	118							
asad_jac.F90	119	REAL, INTENT	(INOUT)	:: ftr(n_poin	ts,jpctr)	! Tracer c	oncs	
asad_mod.F90	120							
asad_posthet.F90	121	REAL, INTENT	(OUT)	:: cdot(n_poi	nts,jpctr)	! Tracer t	endencies	
asad_pris.F90	122							
asad_setsteady.F90	123 🔻 !	Local variab	les					
asad_sparse_vars.F90	124							
asad_spimpmjp.F90	125	INTEGER :: e	rrcode		! Variable p	passed to e	report	
asad_spmjpdriv.F90	126							
asad_steady.F90	127	INTEGER :: j	tr			! Loop va	riable	
asad_totnud.F90 asad_trimol_F90	128	INTEGER :: j	l			! Loop va	riable	