Wet Deposition in UKCA (UM 8.4)

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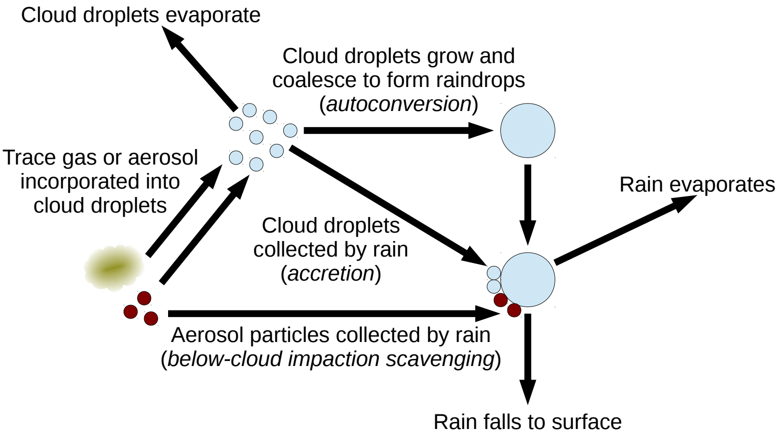
Outline

Introduction

- Wet deposition, by which trace gases and aerosols are removed from the atmosphere by precipitation and deposited at the surface, is one of the major sink processes for soluble compounds in the atmosphere.
- It dominates over dry deposition for soluble trace gases and for all but the coarsest sea-salt and dust aerosols.

Overview


Cloud droplets evaporate
Cloud droplets grow and coalesce to form raindrops (*autoconversion*)
Trace gas or aerosol incorporated into cloud droplets
Rain evaporates
Cloud droplets collected by rain (*accretion*)
Aerosol particles collected by rain (*below-cloud impaction scavenging*)
Rain falls to surface

Trace gases vs. aerosols

- The mechanisms by which trace gases and aerosol are taken up into cloud droplets differ, but once dissolved they are essentially rained out in the same way.

- Nevertheless, due to the separate heritage of the two parts of UKCA, the wet deposition process is implemented quite differently.

Wet deposition of gas-phase chemicals

- Equilibrium assumed between gas phase and solute in cloud droplets, following Henry's law.
- Removal of solute represented as a first-order loss rate proportional to rain rate and fed into the UKCA chemistry solver.
- Formulation based on Giannakopoulos et al. (1999).

Henry's law

- Concentration of dissolved gas is proportional to its partial pressure (with a temperature-dependent coefficient).

$$H_{\text{eff}} = \underbrace{k_{298\text{ K}}}_{\text{Coefficient at 298 K}} \exp\left(-\overbrace{\frac{\Delta H}{R}}^{\text{Temperature dependence parameter}} \left(\frac{1}{T} - \frac{1}{298\text{ K}} \right) \right)$$

- Multiplied by a factor $1 + k_{\text{aq}}/H^+$ to account for dissociation in the aqueous phase, where k_{aq} has a similar temperature-dependent form.
- Applying Henry's law gives the fraction of a trace gas which is dissolved in cloud water.

Linkage to cloud and precip. variables

- Removal rate of the dissolved trace gas is proportional to the diagnosed rain rate R on each level, via a fixed empirical coefficient α:

$$\frac{\mathrm{d}m}{\mathrm{d}t} = -\alpha H_{\mathrm{eff}} m R$$

- No account is taken of the fractional removal rate of cloud liquid water or the cloud cover fraction in the grid box.

Linkage to cloud and precip. variables

- There are coarse temperature-based limits on scavenging in polar regions (no scavenging by ice or snow).
- Convective scavenging is carried out seperately from convective transport, and thus acts on the post-convection environment rather than the rising plume.

Implementation

- Removal rate calculation implemented in `UKCA_WDEPRT`.
- Per-chemistry-scheme configuration in `UKCA_CHEM_`*<scheme>* (e.g. `UKCA_CHEM_STRATTROP`)
- Hand-edit required to set total number of species subject to wet deposition (`JPDW`).

Configuration: selecting species

In `UKCA_CHEM_`*<scheme>* (e.g. `UKCA_CHEM_STRATTROP`):

- Count of species subject to wet deposition, e.g.:

```
INTEGER, PARAMETER, PUBLIC :: nwet_st_aer = 34
```

- Switch to enable wet deposition for a given species, e.g.:

```
TYPE(CHCH_T), PUBLIC :: chch_defs_strattrop_aer(1:87)=(/ &
...
chch_t(3,'O3   ', 1,'TR   ','Ox   ', 1, 1, 0),             &
chch_t(4,'N    ', 1,'TR   ','NOx  ', 0, 0, 0),             &
...
  /)
```

Configuration: Henry's law coefficients

- Henry's law coefficients, e.g.:

```
REAL :: henry_defs_strattrop_aer(1:6,1:nwet_st_aer)=RESHAPE((/
!     1   O3
 0.1130E-01, 0.2300E+04,  0.0000E+00, 0.0000E+00,  0.0000E+00, 0.0000E+00,&
...
!    12   HCl
 0.1900E+02, 0.6000E+03,  0.1000E+05, 0.0000E+00,  0.0000E+00, 0.0000E+00,&
...
!     6   H2O2
 0.8300E+05, 0.7400E+04,  0.2400E-11,-0.3730E+04,  0.0000E+00, 0.0000E+00,&
...
!    31   SO2
 0.1230E+01, 0.3020E+04,  0.1230E-01, 0.2010E+04,  0.6000E-07, 0.1120E+04,&
...
  /)
!   k_298       -DH/R       k_298       -DH/R       k_298       -DH/R
! Main values for H_eff      Values for k_aq         Values for k_aq
!                           (1st dissociation)      (2nd dissociation)
```

Hand-edit

- Unfortunately, the count of species subject to wet deposition is also included in a namelist, as well as directly in the source code, and these values **must** be kept in sync.
- If the value in the source code is changed, the one in the namelist can be updated via a hand-edit, e.g.:

set_jpdw_<*NN*>.ed

```
ed CNTLATM <<\EOF
/JPDW/c
 JPDW = <NN>,
.
wq
EOF
```

Wet deposition of aerosol particles

Aerosol particles can be removed by precipitation in three ways:

nucleation scavenging where aerosol particles act as cloud condensation nuclei (CCN) or ice nuclei (IN) for droplets or ice crystals which later form precipitation;

in-cloud impaction scavenging where aerosol particles are collected by impaction with cloud droplets or ice crystals which later form precipitation (not included in the model);

below-cloud impaction scavenging where aerosol particles are collected by impaction by falling precipitation.

Nucleation scavenging

- Aerosol particles are incorporated into cloud droplets when they act as CCN (*activation*).
- Although (as we'll see later) `UKCA_ACTIVATE` calculates exactly which parts of the aerosol population act as CCN, this has not yet been coupled with the scavenging scheme, which currently uses a simpler approach.

Nucleation scavenging (large-scale): activation

- Based on the approach of GLOMAP-bin (Spracklen et al., 2005), soluble particles larger than a fixed critical wet radius are assumed to act as CCN. This radius is set to 103 nm in `UKCA_SCAVENGING_MOD`:

```
! radius cutoff for activation
REAL, PARAMETER :: nscavact = 103.0e-9
```

- This is translated into the modal scheme as all of the coarse mode, none of the nucleation mode, and the upper portions of the Aitken and accumulation modes.

Nucleation scavenging (large-scale): activation

- This gives the fractions of number ($f_{n,i}$) and mass ($f_{m,i}$) in each mode i (in the cloudy fraction of the grid box) which are dissolved and thus susceptible to wet deposition.

- There is an alternative option to use the fixed scavenging ratios for each mode from ECHAM5–HAM (Stier et al., 2005), though this is rarely used.

Nucleation scavenging (large-scale): removal

- The number and mass are then removed at the same fractional rate as the cloud water itself is removed as precipitation:

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = f_{\mathrm{n},i} C_\mathrm{l} \frac{n_i}{q_\mathrm{cl}} \frac{\mathrm{d}q_\mathrm{cl}}{\mathrm{d}t} \qquad \text{for each mode } i$$

$$\frac{\mathrm{d}m_{i,j}}{\mathrm{d}t} = f_{\mathrm{m},i} C_\mathrm{l} \frac{m_{i,j}}{q_\mathrm{cl}} \frac{\mathrm{d}q_\mathrm{cl}}{\mathrm{d}t} \qquad \text{for each mode } i \text{ and component } j$$

where C_l the liquid cloud fraction in the grid box.

Nucleation scavenging (large-scale): removal

- The removal rate of cloud water is calcluated as the sum of autoconversion (PRAUT), accretion by rain (PRACW) and riming by ice and snow (PIACW+PSACW), based on diagnostics from the large-scale precip. scheme (UMDP 26):

$$-\frac{\mathrm{d}q_{\mathrm{cl}}}{\mathrm{d}t} = \mathtt{PRAUT} + \mathtt{PRACW} + \mathtt{PIACW} + \mathtt{PSACW}$$

- These are added together in UKCA_AERO_CTL before being passed to the scavenging routine (UKCA_RAINOUT).

Nucleation scavenging (large-scale): bugs

- Be aware that there has been a bug making the large-scale precip. diagnostics (and hence the scavenging rates) incorrect in UM 8.4 GA4 jobs.

- The model is largely tuned to compensate, but if you're working on these processes you should probably make sure to include the bug fix and associated re-tuning.

Nucleation scavenging (large-scale): caveats

- No more than 90% by number of a given mode may be removed in a timestep.
- For very low liquid water contents, a fixed removal timescale is applied instead to avoid numerical instability.
- Below 258 K, all particles in the insoluble modes are also susceptible to wet deposition (but by rain only – there is no actual treatment of ice nucleation scavenging yet).

Nucleation scavenging (convective): outline

- Based on Kipling et al. (2013), this operates from within the convection scheme (UMDP 27), removing aerosol as the tracers are transported within the convective updraught.
- All of the soluble accumulation and coarse modes, none of the nucleation mode and a configurable fraction (default 50%) of the soluble Aitken mode considered to be dissolved.
- The dissolved aerosol is removed at the same fractional rate as condensate is converted to precipitation within the convective plume.

Nucleation scavenging (convective): outline

- Similar formulation to the large-scale scheme, but in flux rather than mixing-ratio form. As the convective parcel ascends, the aerosol number within it is reduced by:

$$\frac{\mathrm{d}\,n_i^{(\mathrm{p})}}{\mathrm{d}z} = -\frac{f_{\mathrm{n},i}^{(\mathrm{p})}\, g n_i^{(\mathrm{p})}}{M q_{\mathrm{cl}}^{(\mathrm{p})}} \frac{\mathrm{d}\,P}{\mathrm{d}z} \qquad \text{for each mode } i$$

  where $^{(\mathrm{p})}$ denotes in-parcel properties, M is the convective mass flux, $\frac{\mathrm{d}P}{\mathrm{d}z}$ is the rate at which precipitation is formed, and $f_{\mathrm{n},i} = 0$, 1 or 0.5 depending on the mode.

- Each mode is scavenged uniformly, so the mass per particle is unchanged.

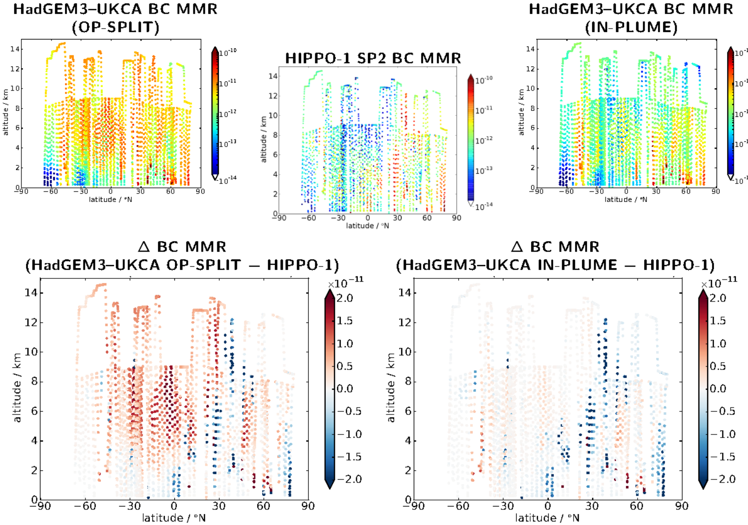
Nuc. scavenging (convective): implementation

- Implemented as UKCA_PLUME_SCAV in UKCA_SCAVENGING_MOD.
- Called from CONVEC2 at each level within the body of the convection scheme, using in-plume variables, rather than from anywhere within UKCA_MAIN1 (which sees only the end-of-timestep environment).
- Usual UKCA/GLOMAP-mode variables therefore not available, and logic is required to identify the number and mass tracers from the combined UM tracers array.

Nuc. scavenging (convective): implementation (2)

- `UKCA_SCAV_INIT` sets up the mappings required to identify the tracers, and is called from `UKCA_INIT`.
- `UKCA_CALC_AQUEOUS` calculates the fraction of each tracer which is susceptible to wet deposition.
- `UKCA_PLUME_SCAV` calls this and calculates the rate at which each tracer is removed from the plume at this level.
- Note that diagnostics for convective removal rates are currently missing.

Why is in-plume scavenging important?



UM 7.3 N96L38

Kipling et al. (2013, ACP)

Below-cloud impaction scavenging: rain

- This follows Slinn (1984), based on a 2D look-up table of scavenging efficiencies for different aerosol and raindrop sizes.
- Aerosol modes are treated as monodisperse at their geometric-mean wet radius.
- Raindrops are divided into 7 bins assuming a Marshll–Palmer distribution.

Below-cloud impaction scavenging: snow

- This is implemented as a power law for each mode following Wang et al. (2011), where the fraction removed from each mode m is:

$$k_m = \overbrace{a_m}^{\text{prescribed coefficient and exponent for each mode}} \underbrace{P}_{\text{total (LS+conv.) snowfall rate}}{}^{\overbrace{b_m}}$$

Below-cloud impaction scavenging: implementation

- Code for both rain and snow is in `UKCA_IMPC_SCAV`.
- Look-up table for rain is in `UKCA_MODE_SETUP`.
- Large-scale and convective precip. are handled similarly, except that they are assumed to apply over 100% and 30% of the grid-box respectively (the large-scale rain fraction diagnostic is not used).

What's missing?

- Re-release of scavenged trace gases and aerosol particles when precipitation evaporates.
- In-plume convective scavenging for gas phase.
- Use of liquid water content and cloud fraction for gas phase.
- Removal of trace gases by ice-phase precipitation.
- Coupling between aerosol activation and scavenging.
- In-cloud impaction scavenging of aerosol.
- Scavenging of ice nuclei.
- Prognostic in-cloud/interstitial aerosol split.
- Misc. inconsistencies between gas phase and aerosol.

A final note on branches

- A number of the features described were not yet in the UM trunk at 8.4, although they are in the `vn8.4_UKCA` package branch.
- The description in the 8.4 version of UMDP 84 describes the trunk rather than the branch, so you may be better referring to the 9.2 version in this instance.

References

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