Interaction of UKCA aerosols with radiation: UKCA_RADAER

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The UK Chemistry and Aerosol (UKCA) model includes an atmospheric aerosol scheme called UKCA-MODE. This new scheme is very different from the CLASSIC aerosol schemes which have been used in the Unified Model so far. Those differences impact the way aerosols interact with radiation to provide scattering and absorption of radiative fluxes (aerosol direct effect) and aerosol optical depth diagnostics. This documents details how the interaction of UKCA-MODE aerosols with radiation, called UKCA_RADAER, differs from the CLASSIC interaction. The implementation of UKCA_RADAER within the Unified Model is then described.

Contents

1 Interaction of aerosols with radiation

1.1 Aerosol optical properties in the radiation scheme

The Unified Model radiation scheme divides the shortwave and longwave spectra into wavebands. Consequently, optical properties of atmosphere constituents, such as gases and aerosols, have to be integrated across those wavebands from the original monochromatic calculations. 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 (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*.

1.2 CLASSIC aerosols

The CLASSIC aerosol schemes interactively simulate the dry aerosol mass of a selection of aerosol species. For each species, the mass is distributed into one or two optically-active modes. Each mode is associated with a prescribed lognormal size distributions (modal radius and standard deviation), a set of wavelength-dependent complex refractive indices, and an estimate of the increase in aerosol size with relative humidity (hygroscopic growth). Since those parameters are prescribed, the monochromatic aerosol optical properties can be computed offline by Mie calculations and averaged across shortwave and longwave waveband. Average values are then stored into blocks 11 of the Unified Model spectral files, with one block for each mode of each aerosol species. Within the radiation code, block 11 acts as a look-up table providing the appropriate aerosol properties, depending on the aerosol species included and the simulated relative humidity.

1.3 UKCA-MODE aerosols

The UKCA-MODE aerosol scheme not only simulates the dry aerosol mass, but also the mass of water attached to the aerosol, and the aerosol number concentrations. The total aerosol mass and number is distributed across 7 modes, characterised by their solubility and the range of particle sizes they cover. Each mode is made of a mixture of several aerosol chemical compo-

Mode name	Size range (nm)	Composition	Solubility
Nucleation soluble	$\overline{r} < 5$	SU	Yes
Aitken soluble	$5 < \overline{r} < 50$	SU, BC, OC	Yes
Aitken insoluble		BC, OC	No
Accumulation soluble	$50 < \overline{r} < 500$	SU, BC, OC, SS, DU	Yes
Accumulation insoluble		DU	No
Coarse soluble	$500 < \overline{r}$	SU, BC, OC, SS, DU	Yes
Coarse insoluble		DU	No

Table 1: *The seven modes in the UKCA-MODE aerosol scheme, their size ranges and their components. Components are sulphate (SU), black carbon (BC), organic carbon (OC), sea salt (SS) and dust (DU).* $\overline{r}$ *is the geometric mean radius (nm) of aerosol particles.*

nents, as listed in Table 1. Modal aerosol size distributions are assumed to be lognormal, with the mean radius being interactively derived from the modal mass and number, and the standard deviation being prescribed at 1.59 for nucleation, Aitken, and accumulation modes, and 2 for coarse modes. The nucleation mode contains particle which are too small to be optically active and is therefore neglected by UKCA_RADAER.

Compared to CLASSIC, the UKCA-MODE scheme introduces three important changes which are relevant to the radiation scheme:

1. The mean radius of the modal size distributions varies interactively;
2. The modal refractive index varies with the internal composition of the mode;
3. The amount of aerosol water in each soluble mode varies interactively.

Consequently, it is not possible to obtain the aerosol optical properties through offline calculations. They have to be computed at runtime, but doing monochromatic Mie calculations at runtime is expensive. Instead, UKCA_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:

1. to compute the modal refractive index out of the simulated chemical composition of each mode;

2. to obtain the monochromatic properties from the look-up tables at selected wavelengths within each shortwave and longwave wavebands;

3. to integrate across each waveband to obtain the waveband-averaged optical properties, which can be used by the radiation code.

In addition to the look-up tables, UKCA_RADAER requires some ancillary data describing the different aerosol components that can belong to a mode, as well as parameters for the integration across wavebands, such as the number and wavelength of the integration points.

The following sections describe the look-up tables of aerosol optical properties, the file of ancillary data, and the implementation of UKCA_RADAER within the radiation scheme of the Unified Model.

2 Look-up tables of optical properties

2.1 Contents

UKCA_RADAER look-up tables provide monochromatic scattering and extinction coefficients σ_{sca} and σ_{abs} (in m^{-1}), asymmetry parameters g (dimensionless), and volume fractions V_{frac} (dimensionless). These parameters depend on the particle radius r and complex refractive index $m = n_r - i\ n_i$, and radiation wavelength λ. Since aerosols are represented by size distributions instead of a single particle size, parameters provided by Mie calculations have to be integrated over that size distribution:

$$\sigma_{\mathrm{sca}}\,(r,\ \lambda,\ n_{\mathrm{r}},\ n_{\mathrm{i}}) = \int Q_{\mathrm{sca}}\,(r,\ \lambda,\ n_{\mathrm{r}},\ n_{\mathrm{i}})\ \ n(r)\ r^2\ dr \tag{1}$$

where $n(r)$ is the number size distribution (lognormal in UKCA_RADAER) and Q_{sca} is the dimensionless efficiency factor for scattering, obtained by applying Mie theory. Equations for σ_{abs} and g are similar.

Mie theory shows that the optical properties of a spherical aerosol particle depend only on the dimensionless Mie parameter x, defined as

$$x = \frac{2\ \pi\ r}{\lambda} \tag{2}$$

and the complex refractive index. Equation 1 can then be rewritten as

$$\sigma_{\mathrm{sca}}\left(x,\ n_{\mathrm{r}},\ n_{\mathrm{i}}\right) = \int Q_{\mathrm{sca}}\ n(x)\ x^2\ dx \tag{3}$$

$$= \left(\frac{2\ \pi}{\lambda}\right)^2 \sigma_{\mathrm{sca}}\left(r,\ \lambda,\ n_{\mathrm{r}},\ n_{\mathrm{i}}\right) \tag{4}$$

Doing so is interesting since it reduces the number of dimensions in the look-up tables from 4 to 3 by grouping radius and wavelength together. The extra factor introduced by the change of variable, $(2\pi/\lambda)^2$, is only partially accounted for when computing look-up tables. The correction for $(2\pi)^2$ is straightforward, but that for the wavelength cannot be made offline, since wavelengths depend on the decomposition of shortwave and longwave spectra and are only known at runtime. Look-up table values must then be divided by the wavelength (m) before being used in the model.

Finally, look-up tables contain the volume fraction of the dry aerosol. This quantity is needed for converting the scattering and extinction coefficients into specific coefficients, i.e. convert from units m^{-1} to $\mathrm{m}^2\ \mathrm{kg}^{-1}$. Volume fraction V_{frac} only depends on the particle radius or, in our framework, the Mie parameter. It is computed as:

$$V_{\mathrm{frac}}\left(x\right) = \frac{4}{3}\ \pi \int x^3\ n(x)\ dx = \left(\frac{2\pi}{\lambda}\right)^3 V_{\mathrm{frac}}\left(r,\ \lambda\right) \tag{5}$$

Again, the factor introduced by the change of variable is corrected at runtime when the wavelength is known.

2.2 Parameter ranges

Each look-up table entry is computed for discrete values of x, n_r, and n_i. The current dimensions are 51 values for the these three parameters. Values of n_r and n_i are distributed linearly across their range. The distribution of x follows a logarithmic scale.

The range of Mie parameters covered by a look-up table depends on the range of particle radii, given by the UKCA-MODE setup shown in Table 1, and the range of wavelengths, i.e. the shortwave and longwave spectra. The most efficient coverage of the Mie parameter range is achieved by using 4 different look-up tables, tailored for Aitken/accumulation or coarse modes, and shortwave or longwave spectrum, respectively. The ranges of real and

Look-up table	Environment variable	Range of x	Range of n_r	Range of n_i
Accum. mode, SW	UKCAACSW	$4\ 10^{-3}$ – 32	1.25 – 2	0 – 0.6
Accum. mode, LW	UKCAACLW	$4\ 10^{-6}$ – 2	0.50 – 3	10^{-9} – 1
Coarse mode, SW	UKCACRSW	0.3 – 48	1.25 – 2	0 – 0.6
Coarse mode, LW	UKCACRLW	$3\ 10^{-4}$ – 3	0.5 – 3	10^{-9} – 1

Table 2: Minimum and maximum value for Mie parameter x, and real and imaginary parts of the refractive index n_r and n_i in the 4 UKCA_RADAER look-up tables.

imaginary parts of the refractive index are chosen to cover realistic values in the shortwave and longwave spectrum. Coverage of Mie parameter and refractive index in each look-up table is summarised in Table 2.

2.3 Format

Look-up tables are text files in the Fortran namelist format. The name of the namelist is UKCANML and the variables in the namelist are:

- STDEV: the standard deviation of the lognormal size distribution (for information only, differentiates Aitken/accumulation mode look-up tables from coarse mode look-up tables);
- X_MIN and X_MAX: the minimum and maximum values for the Mie parameter in the look-up table;
- N_X the maximum array index for the Mie parameter. Note that array indices start at zero in the look-up tables;
- NR_MIN, NR_MAX, N_NR: as above for the real part of the refractive index;
- NI_MIN, NI_MAX, N_NI: as above for the imaginary part of the refractive index;
- UKCA_ABSORPTION: Absorption coefficient as a function of Mie parameter and complex refractive index. Uncorrected for the multiplication factor in Equation 3;

- UKCA_SCATTERING: As above for the scattering coefficient;
- UKCA_ASYMMETRY: As above for the asymmetry parameter;
- VOLUME_FRACTION: The aerosol volume fraction as a function of Mie parameter.

Current UKCA_RADAER look-up tables are on the supercomputer at *~hadnd/ukca* and named *nml_ac_sw*, *nml_cr_sw*, *nml_ac_lw*, *nml_cr_lw* where *ac* stands for accumulation mode and *cr* for coarse mode.

3 File of pre-computed values

UKCA_RADAER uses a file of pre-computed values containing ancillary data used to provide refractive indices for all aerosol components that can belong to a mode, and information about integration points for the integration across spectral wavebands. Some of the contents of the file depend on the spectral files of the radiation scheme. The code checks for minimal consistency between files. The file of pre-computed values is in a human-readable text format. It contains:

- The number of integration points within a waveband. Currently set to 6;
- The weight of each integration points in the integral. Currently unused, as a trapezoidal integration is coded explicitly;
- For each spectrum (shortwave, longwave):
  - The number of wavebands. Must match the settings in the spectral files;
  - The dimensions of the corresponding UKCA_RADAER look-up tables for accumulation- and coarse-mode aerosols;
  - For each waveband:
    - A reminder of the waveband boundaries (for information only);
    - The wavelengths of the integration points;
    - The solar irradiance (shortwave) or Planckian function (longwave) at this wavelength;

    - The integrated solar irradiance (shortwave) or Planckian (longwave) across the waveband;
    - For each aerosol component, the real and imaginary part of the refractive index at integration points. Components currently included are sulphate, black carbon, organic carbon, sea-salt, mineral dust, secondary organic carbon, and water;

- Variables needed for the computation of the aerosol optical depth:
  - Number and values of wavelengths where the optical depth is computed;
  - For each aerosol component (as listed above), the value of the real and imaginary part of the refractive index at the optical depth wavelengths.

The current file of UKCA_RADAER pre-computed values is on the supercomputer at *~hadnd/ukca/pcalc_hadgem1_5.ukca* and corresponds to the standard spectral files used by HadGEM (6 shortwave wavebands, 9 longwave wavebands).

4 UKCA_RADAER in the Unified Model

UKCA_RADAER is associated with the model switch *L_UKCA_RADAER*. When the model switch is set to true, the model will try to read the UKCA_RADAER input files, get data from UKCA-MODE, and compute UKCA-MODE aerosol optical properties within the Unified Model radiation scheme.

4.1 Input of external files

The 4 UKCA_RADAER look-up tables and the file of pre-computed values are loaded at the start of a model run, in routine *initphys*, just after the input of the spectral files of the radiation scheme.

The 4 look-up tables are loaded by routine *ukca_radaer_read_luts* which calls routine *ukca_radaer_lut_in* for each look-up table. Paths to the look-up tables are associated with environment variables UKCAACSW, UKCACRSW, UKCAACLW, UKCACRLW. The contents of the look-up tables are stored in module *ukca_radaer_lut_mod*. The type of the look-up tables is the derived

type (or structure) *ukca_radaer_tlut* as declared in module *ukca_radaer_tlut_mod*.

The file of pre-computed values is loaded by routine *ukca_radaer_read_precalc*. Upon input, basic consistency between that file and the spectral files is checked by ensuring that the number of spectral waveband is the same in all files. Spectral file contents are accessed by routine *ukca_radaer_get_specinfo*. Path to the file of pre-computed values is given by environment variable UKCAPREC. Pre-computed values are stored in a structure defined and declared in module *ukca_radaer_precalc_mod*.

4.2 Coupling with UKCA-MODE

UKCA_RADAER requires input from UKCA-MODE. The input needed resides in UKCA sections 34 (prognostic variables) and 38 (diagnostic variables). Input fields are:

- Aerosol number concentrations in each mode;
- Mass-mixing ratios of all aerosol components within each mode;
- Modal diameters for dry and, for soluble modes, wet aerosols;
- Modal density;
- Volume of each aerosol component in each mode and, for soluble modes, volume of aerosol water in the mode.

UKCA-MODE data is acquired in *Atm_Step* and is stored into the UKCA_RADAER structure, which is defined by module *ukca_radaer_struct_mod*. When routine *Atm_Step* is first called, routine *ukca_radaer_init* initialises the structure. It lists the STASH items that are needed, depending on the configuration of UKCA-MODE (active modes, active components within each mode). *ukca_radaer_init* exists in two version: the full version is compiled when section A34_1A is defined, i.e. when UKCA-MODE is available. An error version is compiled when section A34_0A is defined and causes model failure, as UKCA_RADAER cannot be used without UKCA-MODE.

The data itself is obtained by routine *ukca_radaer_get*. When it is first called, it scans D1 looking for the STASH items listed by *ukca_radaer_init*. Halo support is automatic, and the routine also checks that the input STASH

fields have the expected dimensions and shape. If all required items are found, it transfers the UKCA-MODE data to the UKCA_RADAER structure.

4.3 Within the radiation scheme

The UKCA_RADAER structure is passed down the calling tree to the radiation scheme, where relevant data is copied into local arrays, reshaped following the conventions used in the radiation scheme, as is also done for CLASSIC aerosols.

The actual interaction between UKCA-MODE aerosols and radiation happens in routine *flux_calc*. First, the UKCA-MODE data is processed by *ukca_radaer_prepare*. The routine computes the modal mass-mixing ratio by simply adding the component mass-mixing ratios together. It also converts the modal molecular concentrations to number concentrations (particles per m^{-3}).

The actual interaction can now take place. Waveband-averaged optical properties of UKCA-MODE aerosols are computed by routine *ukca_radaer_band_average*. Results are transferred to routine *grey_extinction* and influence the calculation of atmospheric fluxes. In addition, modal optical depth diagnostics for UKCA-MODE aerosols are computed, if requested, by *ukca_radaer_compute_aod* for each mode. This is only done in the longwave radiation routine in order to get optical depth calculations in all gridboxes (shortwave radiation is only calculated on lit points). Results are transferred to routine *diagnostics_lw* for copy to STASH.

4.3.1 ukca_radaer_band_average

Routine *ukca_radaer_band_average* performs the waveband averaging of monochromatic optical properties taken from the UKCA_RADAER look-up tables. Calculations are done at all gridboxes and levels where the number concentration exceeds 10^4 particles per m^3. This threshold is introduced for the sake of performance, in order not to compute optical properties in pristine environments, but also because UKCA-MODE does not yield realistic modal diameters at low number concentrations. Optical properties are set to zero (no effect on radiative fluxes) at those points where UKCA_RADAER is not applied.

The routine then loops over wavebands and integration points within wavebands (i.e. wavelengths). In order to access the right look-up table entry, Mie parameters for wet and dry aerosols, and modal refractive index are computed. The modal refractive index is simply the volume-weighted average refractive index of components within that mode, including the water component for soluble modes. Look-up table access is made on a nearest neighbour basis, as interpolation is expensive. The routine selects the look-up table to use, out of the 4 available, depending on the current mode (Aitken/accumulation or coarse) and the current spectrum (shortwave or longwave). Once a look-up table element is located, it is corrected for the wavelength-dependent factor missing from the look-up tables, as described in section 2.1. Scattering and absorption coefficients σ (m^{-1}) are also converted to specific coefficients k ($\mathrm{m}^2\ \mathrm{kg}^{-1}$) following

$$k_{\mathrm{sca}} = \frac{\sigma_{\mathrm{sca}}}{\rho\ V_{\mathrm{frac}}} \tag{6}$$

where

- ρ is the modal density ($\mathrm{kg\ m}^{-3}$);
- V_{frac} is the volume fraction ($\mathrm{m}^3\ \mathrm{m}^{-3}$) of the dry aerosol.

In a given waveband and for a given mode, the waveband-integrated specific scattering and absorption coefficients, denoted k_{sca} and k_{abs} and given in $\mathrm{m}^2\ \mathrm{kg}^{-1}$, are computed as:

$$k_{\mathrm{sca}}\,(\mathrm{mode},\ \mathrm{waveband}) = \frac{\sum_{i=1}^{K} w_i\ E(\lambda_i)\ k_{\mathrm{sca}}(\mathrm{mode},\ \lambda_i)}{\sum_{i=1}^{K} w_i\ E(\lambda_i)} \tag{7}$$

where

- i is the i*th* point of integration within the waveband;
- K is the number of integration points within each wavebands and is currently set to 6;
- λ_i is the wavelength (m) at the i*th* integration point and depends on the waveband and the spectrum. Wavelengths are linearly distributed across the waveband and include both waveband boundaries;

- w_i is the unitless weight of the i*th* point in the integration. A simple trapezoidal rule is currently implemented;
- $E(\lambda_i)$ is the solar irradiance (in the shortwave) or the Planckian function (in the longwave) in Wm^{-2} at the wavelength of the integration point. Monochromatic solar irradiances are taken from Labs and Neckel [1970]. The Planckian function is currently computed for a temperature of 250 K.
- $k_{\mathrm{sca}}(\mathrm{mode},\ \lambda)$ is the monochromatic specific scattering coefficient derived from the look-up tables for that mode and at the wavelength of the integration point.

k_{abs} follows the same equation.

Waveband-averaging is slightly different for the asymmetry parameter, as it has to be weighted by the monochromatic specific scattering coefficient:

$$g\,(\mathrm{mode},\ \mathrm{waveband}) = \frac{\sum_{i=1}^{K} k_{\mathrm{sca}}\,(\mathrm{mode},\ \lambda_i)\ g\,(\mathrm{mode},\ \lambda_i)}{\sum_{i=1}^{K} k_{\mathrm{sca}}\,(\mathrm{mode}, \lambda_i)} \quad (8)$$

$$= \frac{\sum_{i=1}^{K} k_{\mathrm{sca}}\,(\mathrm{mode},\ \lambda_i)\ g\,(\mathrm{mode},\ \lambda_i)}{k_{\mathrm{sca}}\,(\mathrm{mode},\ \mathrm{waveband})} \quad (9)$$

Finally, the routine accounts for the excluded bands (or split bands) sometimes used by the Unified Model radiation scheme in its spectral decomposition (See UMDP 23A, section 2, description of block 14 of spectral files). Not supporting excluded bands would cause a double count of aerosol extinction when that type of bands is used.

Modal optical properties have now been calculated and can be used by the radiation scheme in its computation of radiative fluxes.

4.3.2 ukca_radaer_compute_aod

Routine *ukca_radaer_compute_aod* is similar to *ukca_radaer_band_average*, only simpler. Optical depths are monochromatic: it is therefore unnecessary to average across spectral wavebands. In addition, the asymmetry parameter is not required and is not calculated.