Vertical distribution of climatological aerosols

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The main idea is to distribute 2D mass field provided by climate file to the vertical levels. The amount of aerosols between some layer l and the model top can be described by analitycal function - weight w_l. For Tegen climatology, there are 6 fields containing aerosol optical depth at 550nm (AOD550), while new CAMS climatology is providing vertically integrated mass per unit area for 11 aerosol species.

1 Tegen climatology

In the climate file, there can be AOD550 for 6 Tegen aerosol types. Each of them is activated or deactivated by its own key in the namelist `NAMPHY` (Table 1).

Table 1: List of aerosol types

aerosol field name	**description**	**key for activating**
SURFAEROS.LAND	land	LAEROLAN
SURFAEROS.SEA	sea	LAEROSEA
SURFAEROS.DESERT	dust	LAERODES
SURFAEROS.SOOT	urban	LAEROSO
SURFAEROS.SULFAT	sulfates	LAEROSUL
SURFAEROS.VOLCAN	volcanic	LAEROVOL

Aerosols can be considered as either tropospheric or stratospheric. Land, sea, dust and urban types are mainly found in troposphere, while sulfate and volcanic types are of finer sizes and reaching stratosphere.
Because Tegen climatology was obtained from the long term simulations of aerosol model verified against few measurement sites, additional tuning via background values was necessary to get globally unbiased clearsky fluxes in IFS model. There are three background variables that are converted in `phys_ec/suaerv.F90` from total AOD550 to AOD per pressure thickness of troposhere or stratosphere:

- tropospheric: `PTRBGA=YDERAD%TRBKG/(101325._JPRB-19330._JPRB)`; default value is `TRBKG=0.0534_JPRB`
- stratospheric volcanic (ashes): `PVOBGA=0.007_JPRB  / 19330._JPRB`
- stratospheric sulfuric type: `PSTBGA=YDERAD%STBKG/ 19330._JPRB`; default value is `STBKG=0.0045_JPRB`,

where tropospheric and stratospheric boundary values are 101325 and 19330 Pa, respectively.
Stratospheric volcanic background AOD550 can not be changed, while troposferic and sulfuric background can be modified in the `NAERAD` namelist.
Vertical distribution of 6 Tegen aerosol types is done in the subroutine `phys_radi/radaer.F90`. Output is 3D field `PAER(KLON,KLEV,6)`. To distinguish tropospheric and stratospheric aerosols, special weight `ZAETR` is introduced. It is initialized with 1 at the top of the atmosphere, then as we continue downward we decrease it in every layer without temperature inversion by a factor $(\mathrm{T\_top}/\mathrm{T\_bottom})^{30}$. In that way, it will have value 1 in stratosphere, reaching 0 at the surface (Figure 1).

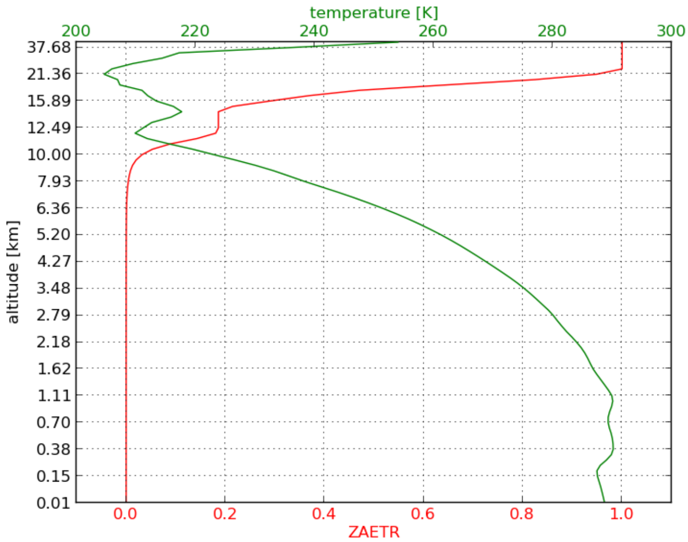


Figure 1: Temperature and ZAETR vertical profiles

Ordering of Tegen aerosols in the array `PAER` is shown in Table 2.

Table 2: List of aerosol types in that order in PAER

N	aerosol	weight	fields if ON	fields if OFF
1	land + sulfates	1-ZAETR	SURFAEROS.LAND + SURFAEROS.SULFAT + PTRBGA	0
2	sea	1-ZAETR	SURFAEROS.SEA	0
3	dust	1-ZAETR	SURFAEROS.DESER	0
4	urban	1-ZAETR	SURFAEROS.SOOT	0
5	sulfates	ZAETR	PVOBGA	PVOBGA
6	volcanic	ZAETR	SURFAEROS.VOLCAN	PSTBGA

Weights for AOD vertical distribution w_l are calculated in the subroutine `phys_ec/suaerv.F90` and it is assumed that aerosol AOD is exponentially decaying with height in troposphere:

$$w_l = \exp\Big(-\frac{z}{H}\Big), \tag{1}$$

where z is height of the model level and H is height scale representing the height at which the normalised cumulative mass distribution reaches the value $1/e$. It depends on aerosol type and spatial distribution.
For Tegen climatology, height scales are defined in `phys_ec/suaerv.F90`: 3km for dust and 1km for sea, land and urban. Stratospheric species (sulfates and volcanic) are accounted for by using assumed constant background values.
If we define σ as $\sigma = \frac{p}{p_{surf}}$, where p is level pressure and p_{surf} surface pressure, we get the following:

$$\sigma = \frac{p}{p_{surf}} = \exp\Big(-\frac{gz}{RT}\Big) = \exp\Big(-\frac{z}{H_{atm}}\Big), \tag{2}$$

where H_{atm} is height scale of the standard atmosphere. In the code it is assumed that $H_{atm} = 8434$m. Then we get

$$\sigma^{\frac{H_{atm}}{H}} = \exp\Big(-\frac{z}{H_atm}\frac{H_{atm}}{H}\Big) = \exp\Big(-\frac{z}{H}\Big), \tag{3}$$

which is the weight (1). It means that the weight w_l can be written as:

$$w_l = \exp\Big(-\frac{z}{H}\Big) = \sigma^{\frac{H_{atm}}{H}} \tag{4}$$

2 CAMS aerosols

Unlike for Tegen climatology, CAMS climatology is providing vertically integrated mass per unit area of 11 aerosol species. Key for activating all 11 CAMS aerosols is `LAEROCMR` in `NAMPHY`. Vertical distribution is done in the routine `phys_radi/radaecmr.F90`. The order of CAMS 2D climatology aerosol types is determined in `mf_phys.F90`. It is crucial to correctly assign their optical properties stored in the netcdf file (see Subsection 2.1) via namelist variable `MAP_AERO_GFL2NC` in `NAMAERO`:

```
MAP_AERO_GFL2NC=-1,-2,-3,1,2,3,-4,10,11,11,-5,
```

Negative sign is indicating hydrophilic types.
Ordering, names, description and `MAP_AERO_GFL2NC` values of the 11 aerosol fields are shown in Table 2.

Table 3: List of aerosol types

N	field name	description	NAMAERO value
1	SURFAEROCMS.SS1	sea salt, small	-1
2	SURFAEROCMS.SS2	sea salt, medium	-2
3	SURFAEROCMS.SS3	sea salt, large	-3
4	SURFAEROCMS.DD1	desert dust, small	1
5	SURFAEROCMS.DD2	desert dust, medium	2
6	SURFAEROCMS.DD3	desert dust, large	3
7	SURFAEROCMS.OM1	organic matter, hydrophilic	-4
8	SURFAEROCMS.OM2	organic matter, hydrophobic	10
9	SURFAEROCMS.BC1	black carbon, hydrophilic	11
10	SURFAEROCMS.BC2	black carbon, hydrophobic	11
11	SURFAEROCMS.SU	sulfates	-5

2.1 Netcdf file

Aerosol optical properties are read from the netcdf file in the subroutine `suaero.F90`. File can be found on belenos: `/home/gmap/mrpm/masekj/const/aero/aerosol_ifs_rrtm_46R1_with_NI_AM.nc`
With the command `ncdump -h filename.nc`, one can see all the variables and description of all aerosol types available. There are 14 hydrophobic and 10 hydrophilic types. Their list with description and reference is presented here:

HYDROPHOBIC

1 Desert dust, bin 1, 0.03-0.55 micron, (SW) Dubovik et al. 2002 (LW) Fouquart et al. 1987

2 Desert dust, bin 2, 0.55-0.90 micron, (SW) Dubovik et al. 2002 (LW) Fouquart et al. 1987

3 Desert dust, bin 3, 0.90-20.0 micron, (SW) Dubovik et al. 2002 (LW) Fouquart et al. 1987

4 Desert dust, bin 1, 0.03-0.55 micron, Fouquart et al 1987

5 Desert dust, bin 2, 0.55-0.90 micron, Fouquart et al 1987

6 Desert dust, bin 3, 0.90-20.0 micron, Fouquart et al 1987

7 Desert dust, bin 1, 0.03-0.55 micron, Woodward 2001, Table 2

8 Desert dust, bin 2, 0.55-0.90 micron, Woodward 2001, Table 2

9 Desert dust, bin 3, 0.90-20.0 micron, Woodward 2001, Table 2

10 Hydrophobic organic matter, OPAC (hydrophilic at RH=20%)

11 Black carbon, OPAC

12 Black carbon, Bond and Bergstrom 2006

13 Black carbon, Stier et al 2007

14 Stratospheric sulfate (hydrophilic ammonium sulfate at RH 20%-30%)

HYDROPHILIC

1 Sea salt, bin 1, 0.03-0.5 micron, OPAC

2 Sea salt, bin 2, 0.50-5.0 micron, OPAC

3 Sea salt, bin 3, 5.0-20.0 micron, OPAC

4 Hydrophilic organic matter, OPAC

5 Ammonium sulfate (for sulfate), GACP Lacis et al

6 Secondary organic aerosol - biogenic, Moise et al 2015

7 Secondary organic aerosol - anthropogenic, Moise et al 2015

8 Fine mode Ammonium sulfate (for ammonia), GACP Lacis et al

9 Fine mode Nitrate, GLOMAP

10 Coarse mode Nitrate, GLOMAP

It should be mentioned that hydrophobic stratospheric sulfate (#14) is obtained as the lowest relative humidity bin of hydrophilic ammonium sulfate (#5).

2.2 Gamma distribution

Piotr Sekula discovered that vertical distributions for some aerosol types do not have maximum at the surface but near the planetary boundary layer top. This means that previously used weights for vertical distribution (4), which assume exponential decay of aerosol mass mixing ratio with height, are not sufficient. For that reason, we assumed new weights following gamma distribution:

$$w_l = (-\ln \sigma_l)^{\beta-1} \sigma_l^{\frac{H_{atm}}{H}} \tag{5}$$

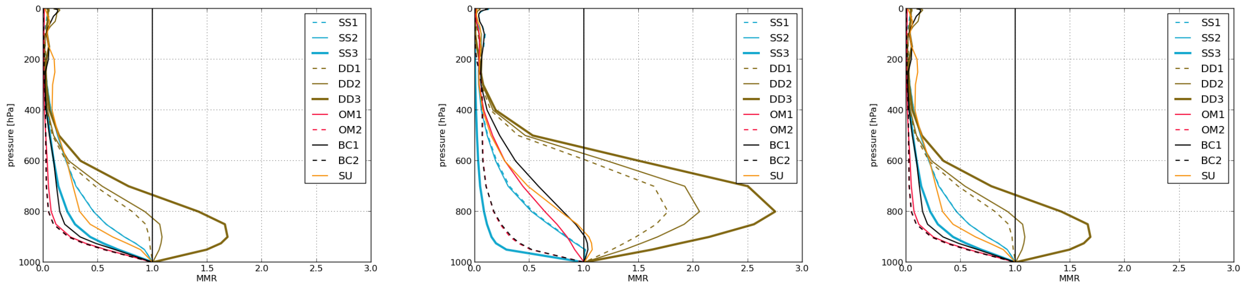
Aerosol dependent height scale H and parameter β can be set in the namelist `NAMAERO`, while H_{atm} is still 8434m. There are two new namelist variables, both arrays of length 25 (maximal possible number of aerosol fields):

- `RAERO_HEIGHT_SCALE` and
- `RAERO_GAMMA_EXP`.

Default values for height scales are set in `suaero.F90`:

- 1000m for sea salt and black carbon
- 2000m for organic matter
- 3000m for dust (can be seasonally dependent for `LDUSEASON=T`)
- 4000m for sulfate.

It is not straightforward to define proper parameter β because it can be very seasonally and based on type dependent.
To examine the best value, we were plotting vertical distribution from CAMS 3D climatology, 20 year averaged fields (2003-2022) over Europe. We were plotting fields for each month and average for the whole year. In Figure 2, vertical CAMS 3D distribution is shown for January, June and average over all months. To emphasize the shape of the distribution, values were normalized with their surface value.



(a) January (b) June (c) all months

Figure 2: Vertical mass mixing ratio distribution of 11 aerosol types, based on CAMS 3D climatology

It can be seen that there is high seasonal variability. For January only desert dust medium and big size have gamma distribution while other species are well described also with exponential function. On the other side, in June not only all three desert dust bins have maximum above the surface but also sea salt small and medium size, hydrophilic black carbon and sulfates.
According to the level where maximum appears for specific aerosol type and month, we prepared a table of parameter β which describes the best distribution for that month and aerosol type.

Table 4: Parameter β in gamma distribution that best describes the vertical distribution, calculated for each aerosol type and for each month. Empty fields mean that the distribution is exponential (β=1)

	1	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**ave**
SS1					1.5	1.5							
SS2					1.5	1.5							
SS3													
DD1		1.5	1.5	1.5	2.0	1.7	2.0	1.7	2.0	1.7	1.7	1.5	
DD2	1.3	1.5	1.5	1.5	2.0	1.7	2.0	1.7	2.0	1.7	1.7	1.5	**1.3**
DD3	1.3	1.5	1.5	1.5	2.0	1.7	1.7	1.7	1.7	1.7	1.5	1.5	**1.3**
OM1													
OM2													
BC1						1.5							
BC2													
SU			1.1	1.1	1.1	1.1	1.1	1.1	1.1				

Impact of gamma distribution is small, so default values for β exponents are set to 1.

2.3 Background values

While for Tegen climatology we use three background values, here we use only two: one tropospheric and one stratospheric. Sulfuric background value has special treatment under key `LAEROVOL=.T.` (see Subsection 2.4). Weight to distinguish troposphere and stratosphere is similar to `ZAETR` (see Section 1). Here it is called `ZMASK_STRATO`, and tropospheric mask is `ZMASK_TROPO=1-ZMASK_STRATO`. Above 10 hPa, both masks are set to zero, ensuring that we do not have any aerosols in mesosphere. The same was done in `radact.F90`.
Both background values can be changed in the namelist `NAMAERO` and are initialized in `suaero.F90` . They are:

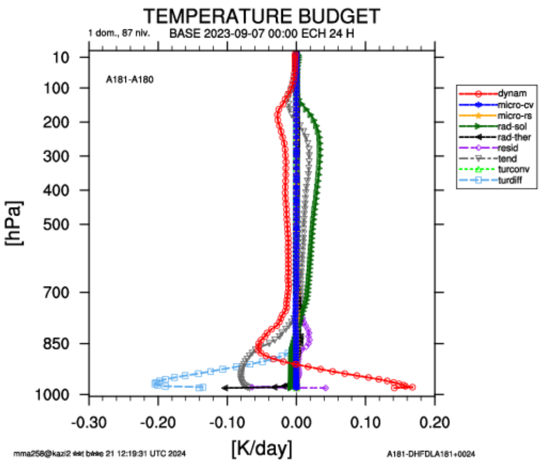
- `RBGST_MMR_OM2` replacing `PVOBGA`
- `RBGTR_MMR_OM2` replacing `PTRBGA`
- `PSTRBGA` will have special treatment in case of `LAEROVOL=.T.` (see Subsection 2.4)

Originally, the idea was to add tropospheric background (Tegen #1) to hydrophobic organic matter (CAMS OM2) and volcanic background (Tegen #5) to sulfate (CAMS SU). After comparing optical properties for Tegen aerosol type #5, sulfates and hydrophobic organic matter, we decided to add both tropospheric and stratospheric background values to hydrophobic organic matter, because its optical properties are more similar to Tegen's #5. For CAMS 2D climatology, hydrophobic organic matter is always on position 8, while for CAMS 3D case (`LAERONRT=.T.`), user should specify the location of hydrophobic organic matter in GFL structure,

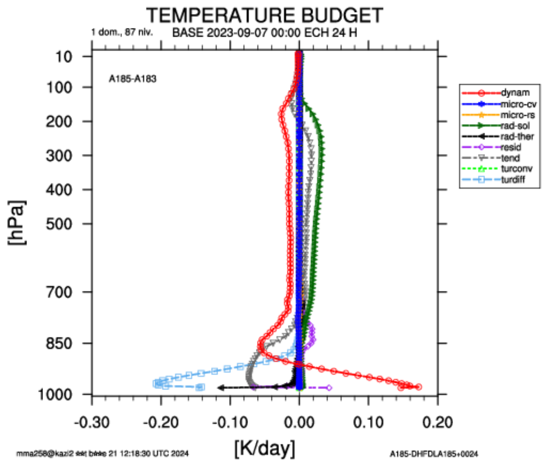
NUMGFL_AERO_OM2.
Initial values from `suaero.F90` were obtained in the following way. Starting point were values from Tegen climatology for tropospheric and volcanic stratospheric background aerosol AOD550. We convert them to mass mixing ratios r. Conversion formula is using Tegen optical properties (EOASA and EODSA) to get braodband AOD from AOD550 and CAMS optical properties from the netcdf file to calculate corresponding broadband delta scaled extinction coefficient k_{ext}^{SW}:

$$r = \frac{(\mathrm{EOASA} + \mathrm{EODSA})\mathrm{AOD550}}{k_{ext}^{SW}\Delta p} \tag{6}$$

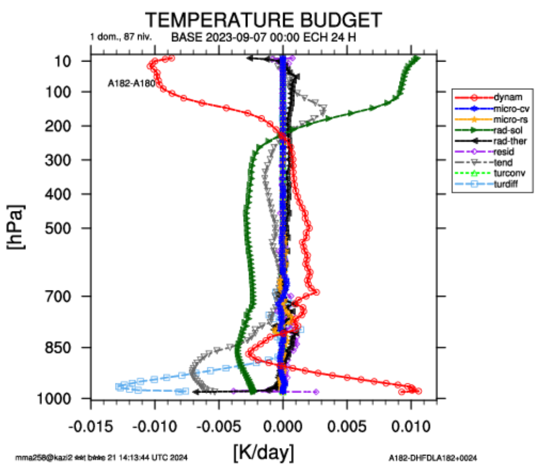
For tropospheric background we use AOD550=PTRBGA and $\Delta p = (101325 - 19330)$Pa, while for stratospheric AOD550=PVOBGA and $\Delta p = 19330$Pa.
Those values were then changed based on DDH plots. We were comparing DDH difference between experiment containing background aerosols and the one without them. The same was done for Tegen and for CAMS case. Background values for CAMS were then scaled in such way to have the similar the impact on shortwave radiation as in the Tegen case.
In Figure 3 are shown DDH plots of 24 hour temperature budget for Tegen (left) and CAMS (right) cases to see impact of tropospheric (top) and stratospheric (bottom) background values. Experiment was run for the clearsky case 07/09/2023. We were focusing primarily on shortwave radiation (green line), but the overall temperature tendency has also similar response (grey line).



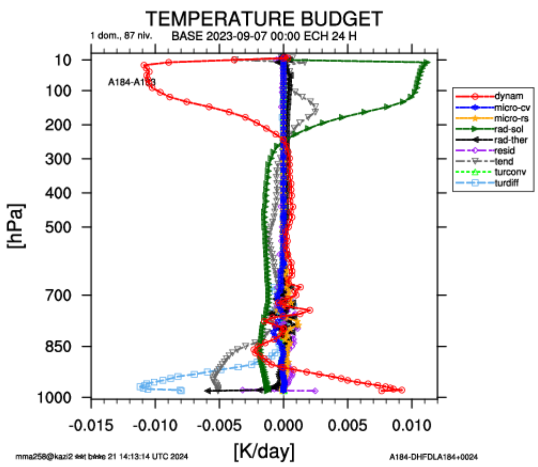
(a) Tegen troposphere



(b) CAMS troposphere



(c) Tegen stratosphere



(d) CAMS stratosphere

Figure 3: Horizontally averaged change in temperature tendency due to the presence of background values.

Since single scattering albedo for hydrophobic organic matter in the shortwave spectrum is 0.85, it means that it is mainly scattering. If we add background aerosols to the troposphere, we have more scattering back to higher levels. This explains heating by shortwave radiation in the higher troposphere when having background

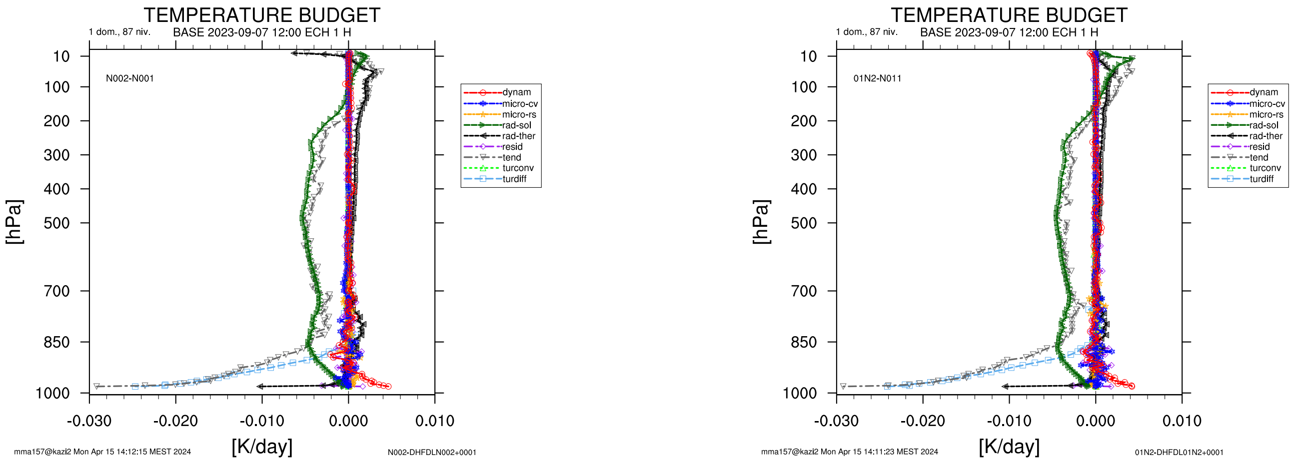
values added (Figure 3a and b). Having more scattering aerosols in stratosphere means less shortwave radiation passing to troposphere. Then we see heating by shortwave radiation in stratosphere and cooling in troposphere (Figure 3c and d). In Figure 3d is also visible jump in the mesosphere due to setting stratospheric mask to 0 for layers higher than 10hPa (which was not the case for Tegen).
Background values are stored to the variable `PAEMMR3D_BG` in `radaecmr.F90`:

```
PAEMMR3D_BG=ZMASK_STRATO*RBGST_MMR_OM2+ZMASK_TROPO*RBGTR_MMR_OM2
```

They are added to aerosol MMR field `PAEMMR3D` in `rad_aer_mmr.F90` to hydrophobic organic matter on position 8 for `LAEROCMR=.T.` and to position `NUMGFL_AERO_OM2` for `LAERNRT=.T.`.

2.4 Volcanic aerosols

In CAMS data, no stratospheric volcanic aerosols are provided. However, global systems driving climate simulations (for example CNRM-ESM2-1 driving ALARO Climate) provide detailed aerosol information. For troposphere, information about aerosols is provided for 11 CAMS aerosol types as either (2D or 3D) MMRs or AOD550. Stratospheric volcanic aerosols are prescribed but only as total AOD550 (FA field `SURFAEROS.VOLCAN`). Based on similar optical properties, they can be represented by CAMS sulfates. Conversion from AOD550 (δ_{550}) to vertically integrated mass is possible if we know its mass extinction coefficient at 550nm, k_{ext}^{550}: $m = \frac{\delta_{550}}{k_{ext}^{550}}$. Since CAMS sulfates are not the same aerosol type as Tegen #6, some tuning of k_{ext}^{550} was needed. It is initialized in `suaero.F90`, but can be modified as namelist `NAMAERO` variable `REXT550_SU`.
In Figure 4 are shown DDH plots for 1 hour integration, starting at 12UTC (to ensure enough sunlight) for the same clearsky case 07/09/2023. Value of AOD550 for `SURFAEROS.VOLCAN` is 0.01.



(a) Tegen (b) CAMS

Figure 4: Horizontally averaged change in temperature tendency due to the presence of stratospheric volcanic aerosols.

In Figure 4, the difference in mesosphere between old Tegen treatment and the new CAMS is visible. In the Tegen case (Figure 4a) there is pronounced cooling to space at the top of the atmosphere, while it is not present in the CAMS case (Figure 4b) due to no presence of aerosols above 10hPa. Another difference is stronger heating by shortwave radiation in stratosphere in CAMS case. This is because Tegen #6 and sulfate types of aerosols do not have identical optical properties. Value of k_{ext}^{550} was tuned based on the impact at the surface. Having volcanic aerosols in stratosphere, less shortwave radiation is reaching troposphere and we see cooling.
In the case of CAMS 2D climatology (`LAEROCMR=.T.`), sulfates are always at the position 11. For CAMS 3D case, `LAERONRT=.T.` option, user should specify the position of sulfates in GFL structure, `NUMGFL_AERO_SU`. Table 5 is showing which fields will be taken in Tegen and in CAMS case for options of `LAEROVOL` switched on and off.

Table 5: Overview of the fields added to existing aerosol types for Tegen and CAMS cases

case	`LAEROVOL=.T.`	`LAEROVOL=.F.`	**added to field**
Tegen	`SURFAEROS.VOLCAN`	`STBKG`	Tegen #6
CAMS 2D	`SURFAEROS.VOLCAN`	0	SURFAEROCMS.SU
CAMS 3D	`SURFAEROS.VOLCAN`	0	GFL field #`NUMGFL_AERO_SU`

Similar to background values, stratospheric volcanic value is stored to the variable PAEMMR3D_VOL in radaecmr.F90:

PAEMMR3D_VOL=RG*PAEVOL*ZMASK_STRATO/(REXT550_SU*ZMASK_STRATO_SUM*ZQD*(PAPRS-PAPRS))

It is added to aerosol MMR field PAEMMR3D in rad_aer_mmr.F90 to sulfates on position 11 for LAEROCMR=.T. and to position NUMGFL_AERO_SU for LAERONRT=.T..

2.5 Call of RADAECMR

Subroutine radaecmr.F90 has to be called two times. First time in case of Tegen or CAMS 2D climatology to perform vertical distribution of 2D climatological fields. Second call is made for case LAERONRT=.T. to get background values which will then be added to ZAEMMR3D aerosol MMR field in subroutine rad_aer_mmr.F90.

```
! Vertical distribution of climatological aerosols
    IF ( ... .AND. (LLAODIN.OR.LAEROCMR) ) THEN
      IF (LLAODIN) THEN
        ! distribute total Tegen AOD vertically
        CALL RADAER( ... )
      ELSEIF (LAEROCMR) THEN
        ! distribute total aerosol mass vertically (CAMS climatology)
        CALL RADAECMR( ..., PAEMASS2D, ZAEVOL, ZAEMMR3D, ZAEMMR3D_BG,ZAEMMR3D_VOL)
      ENDIF
    ENDIF


! Optical properties of CAMS (2D and 3D) aerosols
  IF (LAEROCMR.OR.LAERONRT) THEN
    IF (LAERONRT) THEN
      ZAEMMR3D = PAEMMR3D
      ! get tropospheric and stratospheric background values, add them to 3D MMRs
      CALL RADAECMR( ..., PAEMASS2D, ZAEVOL, ZAEMMR3D, ZAEMMR3D_BG, ZAEMMR3D_VOL)
    ENDIF
    CALL RAD_AER_MMR( ..., ZAEMMR3D, ZAEMMR3D_BG, ZAEMMR3D_VOL)
  ENDIF
```

Figure 5: Simplified code part of APLPAR and APL_AROME where RADAECMR is called

3 Summary

Aerosols in climatological files are given as 2D fields. Vertical distribution of 6 Tegen AOD550 is done in radaer.F90. CAMS climatology contains vertically integrated masses per unit area for 11 aerosol types. They are vertically distributed in the new subroutine radaecmr.F90.
While in radaer.F90 it is assumed that amount of aerosols is decreasing exponentially with height, in radaecmr.F90 we allow the possibility to use more realistic gamma distribution. Based on the investigation of the 3D CAMS climatology, we provide the suggestion of different exponents in the distribution for each aerosol type and month.
Another thing that needed to be adjusted are background values. We decided to keep one tropospheric and one stratospheric background value, while sulfuric background will be treated under the LAEROVOL=.T. case. Their initial values were derived by transforming Tegen background values, projecting them to the corresponding CAMS type (hydrophobic organic matter for tropospheric and stratospheric background) and tuning them to have the similar impact on shortwave radiation as for Tegen climatology.
Altogether there is one new subroutine radaecmr.F90 and 7 new namelist NAMAERO variables:

- RAERO_HEIGHT_SCALE(:)
- RBGST_MMR_OM2
- RBGTR_MMR_OM2
- NUMGFL_AERO_OM2
- NUMGFL_AERO_SU
- REXT550_SU
- RAERO_GAMMA_EXP(:).

Final formula for calculating layer mass mixing ration r_l from the vertically integrated mass m is:

$$r_l = \frac{w_l m g}{\sum_{i=1}^{N} w_i (1 - q_v)_i \Delta p_i} + \mathrm{PAEMMR3D\_BG} + \mathrm{PAEMMR3D\_VOL}, \qquad (7)$$

where g is gravity acceleration, q_v water content and Δp_i pressure difference between adjacent half-levels of the layer i. Second and third terms are tropospheric/stratospheric background values and stratospheric volcanic aerosols.