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Model source code modifications to include the indirect aerosol effect

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List of tables and figures

Terms, definitions and abbreviated terms

The following acronyms have been used across this document:

ACRONYM	FULL TERM
WRF	Weather Research and Forecasting Model
AOD	Aerosol optical depth
Nt_c	Cloud droplet number concentration
MODIS	Moderate Resolution Imaging Spectroradiometer
MERRA	Modern-Era Retrospective analysis for Research and Applications
CORDEX	COordinated Regional climate Downscaling EXperiment

1 Introduction

In this deliverable we describe the process of improving the aerosol indirect effect implementation in Weather Research and Forecasting (WRF) climate model simulations. We present a methodology that enables the proper selection of the cloud droplet number concentration constant, used in a specific microphysics scheme in WRF, to better reflect real life aerosol conditions.

2 Current status of aerosol-cloud interactions in WRF

The WRF code, up to the newest version 4.5, enables the model to access any external aerosol dataset provided by the user (aer_opt=2) and let these aerosols interact with the radiation scheme (Ruiz-Arias et al., 2014). Thus, the model can take into account aerosol-radiation interactions, a component that has been shown to be of considerable importance in climatic simulations due to the long-term trends present in aerosol loads around the globe (Boé et al., 2020).

Indirect aerosol effect (aerosol-cloud interactions) however, is either ignored or taken into account in a simplistic manner by most microphysics schemes in WRF. A very commonly used microphysics scheme is the classic Thompson scheme (mp_physics=8 option) (Thompson et al., 2008). This scheme has been widely used by the WRF community and is currently being used in the new WRF CMIP6-CORDEX simulations that are under production by various institutes.

Indirect effect in the Thompson scheme is implemented crudely. The Thompson microphysics scheme just uses a predefined constant number concentration of cloud droplets (Nt_c) for calculations of rain droplet concentration and also for calculation of cloud particle size. However, the number of cloud droplets heavily depends on the aerosol load present. Therefore, in the Thompson scheme this Nt_c number is not dependent to the actual aerosol load of the domain of the simulation. Moreover, it is characteristic that the user is encouraged to modify this number to better reflect the aerosol conditions. The prescribed number of cloud droplets is set in the code as 100 x10^6 /m^3. Regarding to guidelines within the code this number is better suited for maritime cases while for continental cases a number of 300 x10^6 /m^3 cloud droplets is recommended. The Nt_c constant plays an important role in autoconversion, the process that describes the collision and coalescence between cloud droplets to form raindrops.

As mentioned before, in WRF there is the option of incorporating an external aerosol dataset to be taken into account by the radiation scheme. Thus, we can have a detailed and state of the art dataset to describe aerosol-radiation interactions. We have tried to extract a meaningful number of Nt_c from such an aerosol dataset to be used in the Thompson microphysics scheme. In this way, the aerosol indirect effect is still rudimentary but better suited to the aerosol characteristics of the domain to be simulated, in our case Europe. Moreover, there is enhanced consistency between the aerosol “seen” by the radiation and microphysics schemes.

3 The reference aerosol dataset

We have used a dataset of monthly aerosol optical properties with global coverage that has recently been published specifically to be used in climate model simulations (Solmon et al. 2022). Hereafter, we refer to this dataset as MERRA-CORDEX. This dataset has been created from the NASA MERRA-2 reanalysis of 3-hourly aerosol mixing ratio and relative humidity profiles (GMAO 2015). The MERRA-2 reanalysis is based on the GEOS atmospheric model that is heavily assimilating various observational sources to produce a gridded dataset of physical consistency. The MERA-CORDEX dataset is used as the reference aerosol dataset for the EURO-CORDEX evaluation simulations (Katragkou et al., 2024)

The dataset we use, MERRA-CORDEX, contains aerosol extinction coefficient, single scattering albedo and asymmetry parameter for various spectral bands, vertical layers and aerosol species. There are five aerosol species provided: dust, sea salt, black carbon, organic carbon and sulfates. Moreover, it contains surface pressure data as well as layer thickness and air density for each vertical layer. The 72 vertical layers extend from the surface up to the 0.01hPa level while the horizontal resolution is roughly 0.5^ox0.625^o. It covers the extensive period 1980-2020, sufficient enough to encompass considerable aerosol trends that have been demonstrated to play a significant role in climatic simulations. Aerosol data are provided for 14 spectral bands, ranging from 346nm up to 12195nm. We use data for the visible spectral band centered at 533nm.

4 Calculation of cloud droplet number concentration

4.1 Methodology

Our goal is to translate the aerosol optical depth (AOD) to Nt_c cloud droplet number concentration. There are several empirical relationships between these two variables. Our methodology is based on that of Stevens et al. (2017) where a relationship between anthropogenic AOD at 550nm (mid-visible range) and Nt_c was derived using the MODIS collection 6 satellite data. Even though there were deviations, they found a systematic relationship between the aerosol optical depth of anthropogenic aerosol, AODf, and Nt_c: an increase of Nt_c with an increase of AODf while the increase of Nt_c is more limited the larger the AODf values become. A limitation of the satellite data is that AOD retrievals are problematic above land and limited mainly above the sea.
To describe this behavior, they used the following logarithmic relationship:

$$Nt\_c = a_N ln\left(b_N\left(\tau_a + \tau_{bg}\right) + 1\right) \qquad (1)$$

where a_N, b_N, τ_{bg}, are fitting parameters, τ_a is the fine mode (anthropogenic) AODf and τ_{bg} is a parameter describing background aerosol. These background aerosol describe the contribution of the formation of CCN (cloud condensation nuclei) from natural processes that exist even in the clearest atmospheric conditions. We have experimented with values ranging between 0.02 and 0.08 as stated in (Stevens et al., 2017) and (Fiedler et al., 2017). Results of this sensitivity study are seen in the next section. However, the Nc values derived were quite similar. The AOD used in the above relationship is at the visible 550nm range. As mentioned before the MERRA2 dataset has aerosol info in 14 spectral bands from the visible to the infrared. Thus, we chose the band closest to 550nm, that is number 10 that is centered at 535nm (441-625nm).

Since only anthropogenic aerosol are taken into account by the above equation (1) we also chose to isolate the anthropogenic aerosol component from the MERRA-CORDEX dataset. Thus, from the five available species we take into account sulfates, black carbon and organic carbon since these are primarily due to human sources (Bellouin et al., 2005; Ramanathan et al., 2001). The natural aerosol contribution (dust and sea salt) to the Nt_c is taken indirectly into account by the τ_{bg} tunning parameter. We have however experimented using the entire aerosol load and results were similar to the τ_{bg} approach.

4.2 Calculation of AOD

The MERRA-CORDEX dataset provides extinction coefficients at every vertical level for the five aerosol species mentioned as well as surface pressure, pressure layer thickness and layer air density fields. Since we needed only the anthropogenic aerosol we calculated the overall anthropogenic extinction coefficient by summing the extinction coefficients of organic carbon (OC), black carbon (BC) and sulfates (SU) at every level. The anthropogenic AOD_L for a specific level is thus calculated: AOD_L=(OC+BC+SU)*TH
where TH is the thickness for that specific layer. It is TH=DP/(AIRD*9.81) where DP is the pressure difference and AIDR the air density in said layer. The overall antropogenic AOD is then calculated as the sum of the AOD_L of all vertical layers required:

$$AOD = \sum_{L=i}^{j} AOD_L$$

4.3 Selection of layers

The MERRA-CORDEX vertical layers extend up to the 0.01hPA level, extremely high in atmosphere surpassing not only the troposphere but also the stratosphere. The top-level altitude of the dataset above Europe is around 75km. We are interested in the troposphere since that is where the overwhelming majority of aerosol acting as CCN is taking place. At higher altitudes both aerosol concentration as well as clouds are extremely limited to non-existent. Thus, we experimented with selecting only the aerosol data that are up to 20km, an altitude sufficient to encompass the entire troposphere. This usually corresponds to levels 30 to 33 of the MERRA-CORDEX dataset. However, putting an upper limit to 20km does not make a noticeable difference, since aerosol load up to the 20km altitude is almost identical to the AOD calculated for the entire column up to the 0.01hPa level (Figure1, panels a - b). There is just too little aerosol load in the higher altitudes to make a difference. Therefore, for the Nt_c calculation we use the aerosol load calculated for the entire column.

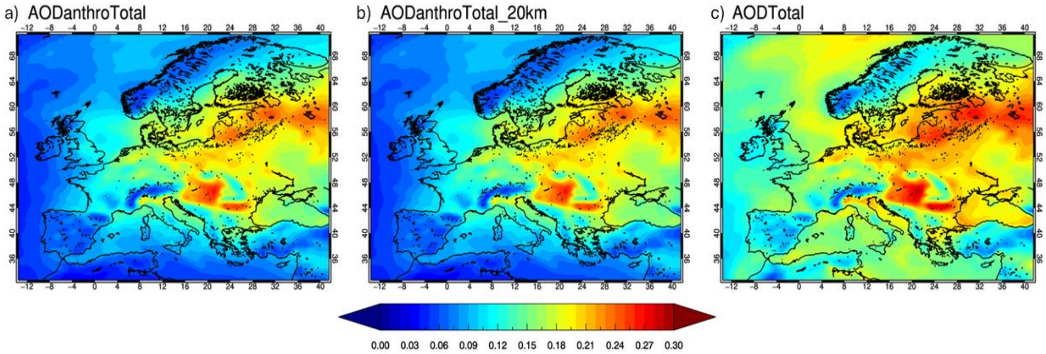

Figure 1: Aerosol optical depth over Europe for January 1980. Taking into account: a) only anthropogenic aerosol (left), b) only anthropogenic aerosol up to 20km altitude (middle), c) all aerosol species (right)

4.4 Results of cloud droplet number concentration calculation

We used the Stevens (2017) method to calculate the Nt_c values over Europe for the entire 1980-2020 period, conducting a sensitivity study of equation (1). Using only the anthropogenic aerosol optical depth we have experimented with various background aerosol values (τ_{bg}) starting from zero background but mainly ranging between 0.02 and 0.08 as stated in (Stevens et al., 2017) and (Fiedler et al., 2017). The calculated Nt_c is larger for a larger τ_{bg} used, however results do not vary greatly and are usually between 70 to 90 x10^6 cloud droplets /m^3 over Europe (Figure2, panels a-b-c). We have also experimented with using all the available aerosol species (anthropogenic + dust + sea salt). In that case we selected a zero background aerosol number (τ_{bg}=0) since theoretically the background aerosol contribution is covered by the natural aerosol species considered. Interestingly, this All species + τ_{bg}=0 approach gives very similar Nt_c results to the Anthropogenic aerosol + τ_{bg}=0.02 approach (Figure 2, panels b-d). This is a strong indication that the τ_{bg}=0.02 background value is a good choice for the European domain. This was also the τ_{bg} value chosen in the Stevens et al. (2017) study.

We have further expanded the sensitivity study by also calculating Nt_c using a different method than equation (1): an empirical relationship used in the ECHAM4 global climate model (Fiedler et al., 2017).

It is: $Nt\_c = \exp\left[\, 5 + 0.3ln\left(\tau_a + \tau_{bg}\right) \right]$ (2)

where τ_a is the again the anthropogenic aerosol AOD and τ_{bg} a parameter describing the background aerosol. Interestingly, Nt_c numbers calculated with equation (2) and using the τ_{bg}=0.02 value (Figure 2 -panel e) are comparable to the Stevens method but clearly present a larger spatial variability. The range of values (around 60 to 100 x10^6 cloud droplets /m^3) is enhanced with the upper limit extending higher and the lower limit extending lower compared to the Stevens method. However, domain averaged Nt_c values do not vary greatly as we can see in next section 4.4.1.

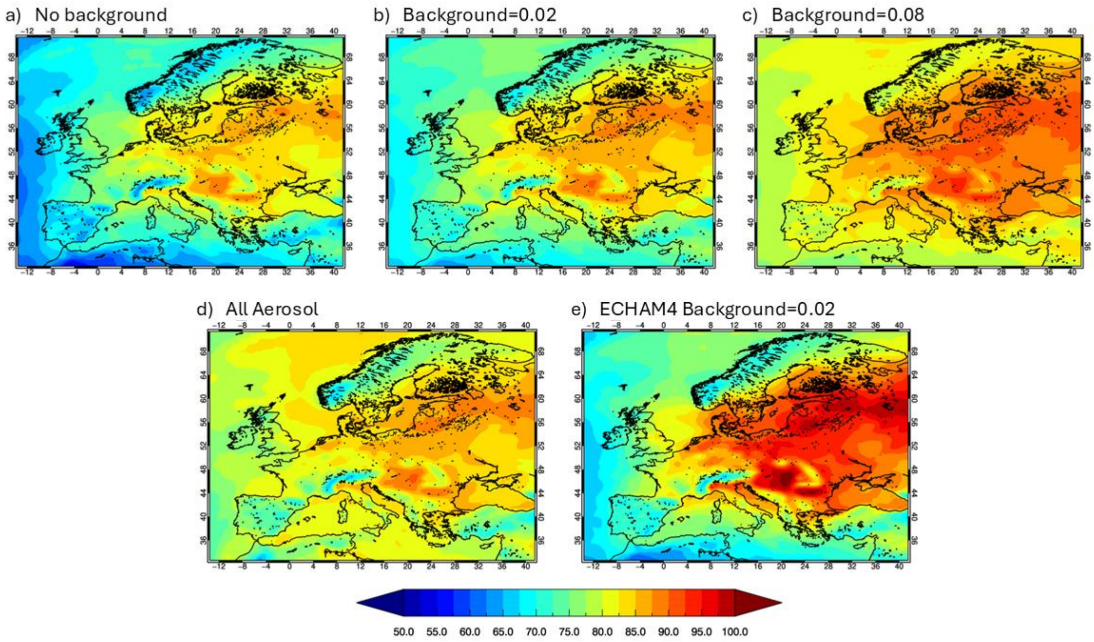

Figure 2: Cloud droplet number concentration (x10^6/m^3) for January 1980 over Europe. Calculated using Stevens 2017 method -relationship (1). Top left (a): Anthropogenic aerosol and no background aerosol (τ_{bg}). Top middle (b): Anthropogenic aerosol and τ_{bg}=0.02. Top right (c): Anthropogenic aerosol and τ_{bg}=0.08. Bottom right (d): All aerosol species and τ_{bg}=0. Calculated using ECHAM4 method -relationship (2). Bottom right: Anthropogenic aerosol and τ_{bg}=0.02

4.4.1 Domain averaged results

For climatic simulations, extending from some months to several years, the proper selection of the Nt_c constant needs to be examined over the entire simulated time period. An example of monthly domain averaged Nt_c values is presented at Table 1 for Europe. Values are given for each month of 1980 as well as for the entire year. The Nt_c values have been calculated using the Stevens (2017) method (columns 3-6) for anthropogenic aerosol with varying background aerosol numbers (columns 3-5) and for all aerosol species without any background aerosol (column 6). Results are also given based on the method used in ECHAM4 model (last column).

Table 1: Monthly average cloud droplet concentration (x10^6/m^3) over Europe for 1980. Columns 3-5: Stevens method using Anthropogenic aerosol and various background aerosol (τ_{bg}) values. Column 6: Stevens method using All aerosol species and thus no background aerosol. Column 7: Method used in ECHAM4 model.

			Stevens 2017 method			ECHAM4 method
Year	month	Anthropogenic τ_{bg}=0	Anthropogenic τ_{bg}=0.02	Anthropogenic τ_{bg}=0.08	All species τ_{bg}=0	Anthropogenic τ_{bg}=0.02
1980	01	75,3	78,1	84,3	81,3	81,1
1980	02	76,9	79,6	85,4	81,7	83,6
1980	03	82,4	84,3	88,8	86,6	91,2
1980	04	82,0	84,0	88,6	86,3	90,8
1980	05	84,6	86,2	90,2	88,2	94,4
1980	06	85,1	86,7	90,7	88,3	95,5
1980	07	86,0	87,5	91,3	88,3	97,0
1980	08	87,2	88,6	92,1	90,0	98,7

1980	09	84,5	86,2	90,2	87,9	94,5
1980	10	79,8	81,9	87,0	84,7	87,1
1980	11	77,1	79,6	85,3	82,3	83,3
1980	12	75,4	78,1	84,2	82,3	80,9
Year average		**81,4**	**83,4**	**88,2**	**85,7**	**89,8**

Overall, the year averaged Nt_c values calculated are relatively close, ranging from 81.4 to 89.8 $x10^6$ droplets $/m^3$. Differences between the various methods exist but are generally restrained. For the Stevens method, as seen in Figure2 the Nt_c values between the Anthropogenic only+τ_{bg}=0.02 approach and the use of All species+ τ_{bg} approach are quite close. Interannual variations do exist but are not considerably high. For example, in the Anthropogenic only+τ_{bg}=0.02 approach the interannual range is between 78.1 and 88.6 $x10^6/m^3$. Interestingly, the ECHAM4 method presents a more pronounced interannual variability (80.9 to 98.7) than the Stevens method.

Climatic simulations usually extend for multiple year periods. Thus, a similar analysis is performed for four different 5-year periods: 1980-1984,1990-1994, 2000-2004, 2010-2014 and 2016-2020. Results for the various approaches using the Stevens method do not vary greatly for the same five-year period (differences less than 8). All methods however, clearly present a declining trend of Nt_c through time. This decline is especially pronounced during the 1980s and 90s and coincides with the drastic reduction of AOD over Europe during that time period (Nabat et al., 2014). Interestingly, the Nt_c declining trend is stronger in the ECHAM4 method.

To sum up, we have seen that the Nt_c values calculated using the various approaches, for monthly, yearly or multiyear averages, do present some small differences. However, what is important to state is that these Nt_c values are in most cases considerably smaller than the default setting of the Thompson scheme, the 100 $x10^6$ cloud droplets $/m^3$ constant value. This difference is even more pronounced for more recent time periods due to the declining Nt_c trend over time. Therefore, if we intend to simulate a five-year period in the 1980s choosing a calculated Nt_c for the Thompson scheme by one of the examined approaches, would result in a 10 to 15% reduction in cloud droplet number concentration compared to the default setting of the Thompson scheme. For a more recent time period (e.g. 2016-2020) the difference would be even higher, around 20 to 30%. Cearly, these are considerable differences that need to be taken into account by modifying the Nt_c constant in the Thompson scheme, if we intend to have a more realistic description of aerosol-cloud interactions in the WRF model.

Table 2: Cloud droplet concentration ($x10^6/m^3$) over Europe averaged for different five-year periods. Columns 3-5: Stevens method using Anthropogenic aerosol and various background aerosol (τ_{bg}) values. Column 6: Stevens method using All aerosol species and thus no background aerosol. Column 7: Method used in ECHAM4 model.

	Stevens 2017 method				ECHAM4 method
Period	**Anthropogenic τ_{bg}=0**	**Anthropogenic τ_{bg}=0.02**	**Anthropogenic τ_{bg}=0.08**	**All species τ_{bg}=0**	**Anthropogenic τ_{bg}=0.02**
1980-1984	83,74	85,49	89,73	87,61	93,29
1990-1994	81,93	83,94	88,62	86,23	90,79

2000-2004	71,36	74,99	82,32	79,27	76,56
2010-2014	71,41	74,97	82,25	78,54	76,42
2016-2020	70,51	74,28	81,83	78,10	75,45

5 Summary and conclusion

In this study we have examined various methods of calculating Nt_c, the cloud droplet number concentration, from AOD data over Europe. We have used a state-of-the-art aerosol dataset constructed specifically to be implemented in climate model simulations. The various methods produced in general similar Nt_c results. However, the calculated Nt_c number concentration results were all considerably smaller than the default constant value used in the Thompson microphysics scheme. This signifies the importance of making changes to this constant to better describe the aerosol-cloud interactions. We prepared a code written in IDL language which can process aerosol information from the MERRA-CORDEX dataset. It can be used to calculate the proper Nt_c value to be replaced in the Thompson scheme, for any given period within the1980-2020 frame. Either for the entire Europe or any sub-domain that we intend to simulate. For the intended climatic simulations described in Task 2.2 we intend to use the Stevens method with the anthropogenic aerosol + τ_{bg}=0.02 approach since it produces results close to the ensemble average of all the approaches used.

6 Code example

Below we present part of the code writer in IDL that calculates the cloud droplet concentration based on the MERRA-CORDEX dataset, using the Stevens (2017) approach.

```
PRO Anthro_AOD_files
;program to open original MERRA aerosol files
; and calculate anthropogenic only AOD
dir = '/mnt/meteo_f/ERA5_forcing/MERRA_Aerosol/Anthropogenic_only/'
dirin = '/mnt/meteo_f/ERA5_forcing/MERRA_Aerosol/Original_files/'
dirout='/mnt/meteo_f/ERA5_forcing/MERRA_Aerosol/Anthropogenic_only/Anthro_
AOD/'

year='1980'
year=String(yr)
year=STRTRIM(year,2)   ;trim blank spaces at string!!

;Main month loop
For mm=0,11 do begin ;month loop

mon=['01','02','03','04','05','06','07','08','09','10','11','12']
daystring=['01','02','03','04','05','06','07','08','09','10','11','12','13','14','15','16','17','18','19
```

```
','20','21','22','23','24','25','26','27','28','29','30','31']
;days=[31,28,31,30,31,30,31,31,30,31,30,31]

days=[31,29,31,30,31,30,31,31,30,31,30,31]  ;1980 IS A LEAP YEAR!!!
print,"YEAR",year," ","Month",mon(mm)

;##### Read in AOD file #####
;Opening MERRA data
elcid =
NCDF_OPEN(dirin+"MERRA2_OPPMONTH_wb10."+year+mon(mm)+".nc")   ;
open input
print, "Open file"
NCDF_VARGET, elcid, "lon", lon
NCDF_VARGET, elcid, "lat", lat ; actual lat?

NCDF_VARGET, elcid, "DELP", DP ; pressure difference layer
NCDF_VARGET, elcid, "AIRDENS", AIRD ;air density

NCDF_VARGET, elcid, "EXTBC", EXTBC ; extinction coefficient black carbon
NCDF_VARGET, elcid, "EXTOC", EXTOC ; ... organic carbon
NCDF_VARGET, elcid, "EXTSU", EXTSU ; ... sulphates

NCDF_VARGET, elcid, "EXTSS", EXTSS ; ... sea salt
NCDF_VARGET, elcid, "EXTDU", EXTDU ; ... dust

NCDF_VARGET, elcid, "AOD", aod ;total aod
;NCDF_VARGET, elcid, "time", time
NCDF_CLOSE, elcid

help, aod, lon, lat,dp,aird,extbc
print, "A"

nx = n_elements(lon(*)) ;sthlon
ny = n_elements(lat(*)) ; arithmos gramon
nz = n_elements(DP(0,0,*)) ; levels
print,nx,ny,nz
print,max(DP),min(DP)
print,max(AIRD),min(AIRD)
print,max(EXTBC),min(EXTBC)
print,max(EXTOC),min(EXTOC)
print,max(EXTSU),min(EXTSU)

lev_thick=Dblarr(nx,ny,nz)
altitude=Dblarr(nx,ny)
level20=Dblarr(nx,ny)
AOD_anthro=Dblarr(nx,ny,nz)
AOD_level=Dblarr(nx,ny,nz)
AOD_total=Dblarr(nx,ny)
```

```
AOD_anthro_total=Dblarr(nx,ny)
AOD_anthro_total_20km=Dblarr(nx,ny)
Nt_c=Dblarr(nx,ny)

Nt_cBG1=Dblarr(nx,ny)
Nt_cBG2=Dblarr(nx,ny)
Nt_cALL=Dblarr(nx,ny)

Nt_cECHAM4=Dblarr(nx,ny)
For i=0,nx-1 do begin
 For j=0,ny-1 do begin
  For k=0,nz-1 do begin

     ;Calculate for every grid point and level the AOD
    lev_thick(i,j,k)=DP(i,j,k)/( AIRD(i,j,k)*9.81 )
    altitude(i,j)=total( lev_thick(i,j,*) )

    OCsum=EXTOC(i,j,k)*lev_thick(i,j,k)
    BCsum=EXTBC(i,j,k)*lev_thick(i,j,k)
    SUsum=EXTSU(i,j,k)*lev_thick(i,j,k)

    AOD_anthro(i,j,k)=OCsum+BCsum+SUsum

    SSsum=EXTSS(i,j,k)*lev_thick(i,j,k)
    DUsum=EXTDU(i,j,k)*lev_thick(i,j,k)

    AOD_level(i,j,k)=OCsum+BCsum+SUsum+DUsum+SSsum

  Endfor
 ;Calculate total AOD from all levels
  AOD_total(i,j)=total( AOD_level(i,j,*) )
  AOD_anthro_total(i,j)=total( AOD_anthro(i,j,*) )

     ;calculate levels up to 20km
       hal=0  ;level index
       alt20=0.0
       while alt20 LT 20000 do begin

      alt20=alt20+lev_thick(i,j,nz-1-hal) ;starting from ground (nz) nad going
upwards ,putting nz-1 since idl starts from 0 in arrays
      hal=hal+1

     endwhile
     ;----------------------------

    level20(i,j)=nz-hal
    AOD_anthro_total_20km(i,j)=total( AOD_anthro(i,j,nz-1-hal:nz-1) )
```

```
        print,"strat limit",alt20," anthrototal",AOD_anthro_total(i,j)," anthro up 20km",AOD_anthro_total_20km(i,j)

;calculate cloud droplet density - Stevens 2017
        Nt_c(i,j)=16*ALOG( 1000*AOD_anthro_total(i,j)+1 )

      Nt_cBG1(i,j)=16*ALOG( 1000*( AOD_anthro_total(i,j)+0.02   )+1 ) ;tbg=0.02

      Nt_cBG2(i,j)=16*ALOG( 1000*( AOD_anthro_total(i,j)+0.08   )+1 ) ;tbg=0.08

        Nt_cALL(i,j)=16*ALOG( 1000*( AOD_total(i,j)  )+1 )  ;tbg=0 since it is covered by the inclusion of all aerosol
;Calculate cloud droplet density – ECHAM4 approach
        Nt_cECHAM4(i,j)=exp( 5.0+0.3*ALOG( AOD_anthro_total(i,j)+0.02 ) ) ;ECHAM4 formula with tbg=0.02
  Endfor
Endfor

print,"Altitude"
print,max(altitude),min(altitude)
print,lev_thick(0,0,*)
;-------------------------------------------------------
```

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