Surface In Situ Particle Number Size Distribution (INSITU PNSD) project within AeroCom Phase III:
Description and Model Output Request

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Introduction

The size distribution, including its variability, is the most important property for describing any interaction of an aerosol particle population with its surroundings. In first order, it determines both, the aerosol optical properties quantifying the direct aerosol climate effect, and the fraction of aerosol particles acting as cloud condensation nuclei quantifying the indirect aerosol climate effect. Aerosol schemes of modern climate models resolve the aerosol particle size distribution (APSD) explicitly. In improving the skill of climate models, it is therefore highly useful to confront these models with precision, dry-state APSD data observed at surface stations, which are traceable to standards in the metrological sense.

Corresponding previous work in AeroCom focussed on comparing size-interval integrated, seasonal particle concentrations at selected sites with ensemble model averages to assess overall model skill (Mann et al., Atmos. Chem. Phys., 14, 4679-4713, 2014). The model data had been assembled as all-tracer model output and needed to be interpreted by the analysing scientist in terms of size distribution. A tedious job which limited the use of the AeroCom phase II output. Also – modellers might provide a different originary interpretation of the model data, based on their model structure relating modes, bins, mixing and composition to number size distribution. More and more data have been recently assembled e.g. in the European ACTRIS project and EBAS database (see ebas.nilu.no). A similar problem, the usage of the high quality in-situ optical property data from GAW stations led to the INSITU AeroCom project (see AeroCom wiki page on phase III experiments).

Building on this work, the INSITU PNSD project intends to refine the approach by asking for a more simple output from the models, to facilitate comparing median particle size and integral concentration of fitted modal size distributions and other common size evaluation metrics. It intends to update the previous work based on AeroCom Phase II results to the current Phase III, and complements the INSITU project under way. It will also look at skill differences between models in order to find reasons for matches and discrepancies, will bring attention to the coarse size fraction (D_p > 1 µm) as well as the fine size fraction (D_p < 1 µm). The project and analysis of the new model output requested is organised in 3 tiers: I) Comparison of log-normal fit parameters in the fine particle fraction to data from mobility size spectrometers and detailed interpretation of individual model performances; II) Comparison of scattering Ångström parameter deduced from integrating nephelometer data as indication of modelling skill in the coarse-mode particle fraction; III) Comparison of integrated mass concentration with gravimetric filter samples as indication of modelling skill in the coarse-mode particle fraction.

TIER I: Comparison of Fine Fraction Particle Size Distribution in Size and Concentration

The objective of this task is to compare dry-state (RH < 40%), fine-fraction PNSD data as well as their variability between AeroCom models and surface in situ observations from regionally representative atmospheric monitoring stations. Both, modelled and observed PNSD data will be fitted with log-normal size distribution modes (at least one for 20 nm < Dp < 90 nm, "Aitken-mode" and one for 90 nm < Dp < 300 nm, accumulation mode). The fit parameters of these modes, integral concentration, median diameter, and standard deviation, will be compared between observations and models to quantify model skill not only in particle concentration, but also particle size. Also modal particle volume will be compared to distinguish model skill between sources / sinks, and aerosol processing. The dry aerosol state is requested because these are the thermodynamic conditions at which the aerosol is usually observed at surface monitoring stations for reasons of comparability. The task will focus on comparing monthly and seasonal averages between models and observations, i.e. the exact modelling year for the comparison is of minor importance. For observation data, the comparison will use the most recent years due to an, over time, increasing number of stations. We therefore request model data for one of the AeroCom focus years 2010, 2008, 2006 in this order of preference. A special model output product is needed since particle size distribution so far hasn't been part of the standard set of AeroCom output parameters.

The model output is requested in NetCDF files in the form of binned particle number size distributions with 20 size bins per decade, 60 bins altogether, with bins logarithmically spaced, in the range between 10 nm and 10 μm particle diameter. The particle concentration in each size bin is to be normalised by the logarithmic width of the bin (base-10 logarithm). The output should contain the overall PNSD, but also the mass distributions in the same bins due to sea salt, organic carbon, sulphate, nitrate, elemental carbon, and dust to facilitate search for contributing factors of matches or mismatches. Other particle fractions, e.g. primary particles of unknown composition, shall be grouped into dust, with a comment made in a readme file. The size distributions need be stated for dry particle conditions. This output is requested at the station locations provided in the Annex excel and ascii file of this document. The particle concentrations should be normalised to standard conditions of temperature and pressure (273.15 K, 1013.25 hPa). The time resolution of the output should be daily, with hourly or monthly output being accepted if daily isn't available.

TIER I Outcomes

- Publication quantifying individual fine-range PNSD model skill with respect to modal particle concentration, modal particle volume, and modal median diameter, discriminated by model. Will include investigation into possible reasons for agreements / disagreements.
- Benchmark dataset of in situ surface particle number size distribution for use by modelers in evaluating their runs
- Proposal of specific model runs to track down reasons for agreements / disagreements between models and observations.
- Comparison of model skill between AeroCom Phase II and Phase III.

TIER II: Comparison of Scattering Ångström coefficient as Proxy for Coarse Fraction Particle Size Distribution

Only the fine fraction of the aerosol particle size distribution is currently observed at surface in situ stations with traceable procedures. For evaluating model skill in the coarse range of the PNSD, the scattering Ångström coefficient $\mathring{A}_{sp}$ will be used. The wavelength dependence of the particle scattering coefficient, parameterised by the Ångström coefficient, is a sensitive function of distribution of particle surface between fine and coarse particles. Investigating model skill for $\mathring{A}_{sp}$ will thus serve to evaluate the models' skill in predicting the coarse-range PNSD.

All model output needed for this task is already part of the model output requested for the AeroCom INSITU project. No additional output is requested here in principal, except if the model version changed.

TIER II Outcomes

- Publication quantifying coarse-range PNSD model skill with respect to scattering Ångström coefficient $\mathring{A}_{sp}$ as proxy. Will include investigation into possible reasons for agreements / disagreements.
- Benchmark dataset of in situ surface scattering Ångström coefficient $\mathring{A}_{sp}$ as proxy for coarse –range particle number size distribution for use by modelers in evaluating their models.
- Proposal of specific model runs to track down reasons for agreements / disagreements between models and observations.

TIER III: Comparison of Size-Integrated Particle Mass Concentration as Proxy for Coarse Fraction Particle Size Distribution

The concentrations of particle mass for particles with aerodynamic diameters smaller than 2.5 µm (PM2.5) and 10 µm (PM10) are parameters observed at surface in situ stations with high quality. The difference of PM2.5 and PM10 mass concentrations is a proxy for the particle volume associated with particles in this size interval. Comparing this data to corresponding model output can therefore serve as an alternative proxy for evaluating the models' skill in predicting the coarse-range PNSD. The crossing of number and mass size distributions will also allow interpretation of fine particle size bias in a given model.

The model output for this task is requested in NetCDF files in the form of binned particle mass size distributions (PMSD) with 20 size bins per decade, with bins logarithmically spaced, in the range between 10 nm and 10 µm particle diameter. The particle concentration in each size bin is to be normalised by the logarithmic width of the bin (base-10 logarithm). The output should contain the overall PMSD, but also the sub-size distributions due to sea salt, organic carbon, sulphate, nitrate, elemental carbon, and other components to facilitate search for contributing factors of matches or mismatches. The size distributions need be stated for dry particle conditions. This output is requested at the station locations provided in the Annex of this document. The particle concentrations should be normalised to standard conditions of temperature and pressure (273.15 K, 1013.25 hPa). The time resolution of the output should be daily, with hourly or monthly output being accepted if daily isn't available. Output for the AeroCom focus years 2010, 2008, 2006, in this order, is preferred.

TIER III Outcomes

- Publication quantifying coarse-range PNSD model skill with respect to PM10 – PM2.5 mass concentration as proxy. Will include investigation into possible reasons for agreements / disagreements.
- Benchmark dataset of PM2.5 and PM10 mass concentrations as proxy for coarse –range particle size distribution for use by modelers in evaluating their models.
- Proposal of specific model runs to track down reasons for agreements / disagreements between models and observations.

TECHNICAL MODEL OUTPUT REQUEST for INSITU PNSD AeroCom phase III *Output requests are organized by analysis proposed for each tier.*

TIER I & III: Model output request for dry, in-situ particle number/mass size distribution evaluation at standard conditions of temperature and pressure (273.15 K, 1013.25 hPa)

Variables*:*

- Dry (0% RH), STP (273.15 K, 1013.25 hPa) particle number/mass size distribution between 10 nm – 10 μm, binned, 20 bins per decade, bins logarithmically spaced, concentration in each bin normalised to logarithmic width of bin (base-10 logarithm) $[dN/d\log_{10}D_p]/ [dM/d\log_{10}D_p]$ for:
    - Total number size distribution.
    - Total mass size distribution.
    - Size mass distribution of sea salt.
    - Size mass distribution of organic carbon.
    - Size mass distribution of sulphate.
    - Size mass distribution of nitrate.
    - Size mass distribution of elemental carbon.
    - Size mass distribution of dust.
    - Median diameter of each size bin

Station dimensional output and frequency:

- 2D: *Daily, surface level* @Station locations (see station list attached) of all variables (use stationid as dimension, lat, lon f(stationid)
- *Note: Frequency requirement relaxation: monthly station output is allowed, but not recommended*
- Data dimension of netcdf variables: [time, particle_diameter, stationid]

Years of simulation/emissions*:*

- 2010 (alternatives that are not recommended: 2006, 2008, 2012, 2000)

Variable names:

- <VariableName>:
    - dndlogdaer, dmdlogdaer, dmdlogdss, dmdlogdoc, dmdlogdso4, dmdlogdno3, dmdlogdec, dmdlogddust
- Standard names for these variables respectively
    - log10_size_interval_based_number_size_distribution_of_dried_aerosol_particles_at_stp_in_air
    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_sea_salt_at_stp_in_air

    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_organic_carbon_at_stp_in_air
    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_sulphate_at_stp_in_air
    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_nitrate_at_stp_in_air
    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_elemental_carbon_at_stp_in_air
    - log10_size_interval_based_mass_size_distribution_of_dried_aerosol_particles_due_to_dust_at_stp_in_air

- <VerticalCoordinateType>: “Surface”
- <Period>: ”2010”
- <Frequency>: “daily” (not recommended alternatives: ”monthly”)

Timeline:

- **TIER I** submissions: as soon as possible, best before 30th November 2015.

TIER II: *This output corresponds to the output of the INSITU project, TIER I*

Model output request for dry, in-situ optical parameter evaluation at ambient T,P

Variables*:*

- Dry (0%RH) aerosol extinction @ 550, 440, 870 nm,
- Dry (0%RH) aerosol absorption @ 550, 440, 870 nm
- Dry (0%RH) fine mode (< 1 um diameter) aerosol extinction and absorption @ 550 nm
- Temperature, Pressure, Specific humidity (alternatively relative humidity)

Station dimensional output and frequency:

- 2D: *Daily, surface level* @Station locations (see station list attached) of all variables (use stationid as dimension, lat, lon f(stationid)
- *Note: Frequency requirement relaxation: monthly station output is allowed, but not recommended*
- Data dimension of netcdf variables: [time, stationid]

Years of simulation/emissions*:*

- 2010 (alternatives that are not recommended: 2006, 2008, 2012, 2000)

Variable names:

- <VariableName>: ec550dryaer, abs550dryaer, ec440dryaer, abs440dryaer, ec870dryaer, abs870dryaer, ec550drylt1aer, abs550drylt1aer, asydryaer, temp, hus, pres
  <VerticalCoordinateType>: “Surface”
  <Period>: ”2010”
  <Frequency>: “hourly”, “daily” (not recommended alternatives: “3hourly”,”monthly”)

Timeline:

- **TIER II** submissions: as soon as possible, best before 31st January 2016.

All TIERS

Format: netCDF, see htap format description

File names:
aerocom3_<ModelName>_<ExperimentName>_<VariableName>_<VerticalCoordinateType>_<Peri od>_<Frequency>.nc

Experiment name: <ExperimentName>: "INSITU PNSD"

Data submission procedure:
Via scp or ftp to aerocom-users.met.no server (see AeroCom wiki)

Synergy with other AeroCom experiments:
Simulations for other model intercomparisons (INSITU, HTAP, nitrate, BB experiments…) may be used to provide the specific output requested here. In particular the annual Aerocom_A3_CTRL simulation (suggested at the last AeroCom workshop), with basic output of variables characterizing budgets, optical depth and aerosol surface concentration, its composition and deposition is recommended to be submitted at the same time.

References

Mann, G. W.; Carslaw, K. S.; Reddington, C. L.; Pringle, K. J.; Schulz, M.; Asmi, A.; Spracklen, D. V.; Ridley, D. A.; Woodhouse, M. T.; Lee, L. A.; Zhang, K.; Ghan, S. J.; Easter, R. C.; Liu, X.; Stier, P.; Lee, Y. H.; Adams, P. J.; Tost, H.; Lelieveld, J.; Bauer, S. E.; Tsigaridis, K.; van Noije, T. P. C.; Strunk, A.; Vignati, E.; Bellouin, N.; Dalvi, M.; Johnson, C. E.; Bergman, T.; Kokkola, H.; von Salzen, K.; Yu, F.; Luo, G.; Petzold, A.; Heintzenberg, J.; Clarke, A.; Ogren, A.; Gras, J.; Baltensperger, U.; Kaminski, U.; Jennings, S. G.; O'Dowd, C. D.; Harrison, R. M.; Beddows, D. C. S.; Kulmala, M.; Viisanen, Y.; Ulevicius, V.; Mihalopoulos, N.; Zdimal, V.; Fiebig, M.; Hansson, H. C.; Swietlicki, E.; Henzing, J. S., Intercomparison and evaluation of global aerosol microphysical properties among AeroCom models of a range of complexity. Atmos. Chem. Phys. 2014, 14 (9), 4679-4713.