SPECIAL PROJECT FINAL REPORT

All the following mandatory information needs to be provided.

Project Title:	EC-Earth Atmospheric Composition developments
Computer Project Account:	spgrmyri
Start Year - End Year :	2024 - 2026
Principal Investigator(s)	Stelios Myriokefalitakis
Affiliation/Address:	National Observatory of Athens (NOA), I. Metaxa & Vas. Pavlou, GR-15236 Penteli, Greece
Other Researchers (Name/Affiliation):	Orfeas Karathanasopoulos Giorgos Papangelis

The following should cover the entire project duration.

Summary of project objectives

(10 lines max)

For this special project, we proposed to further develop the EC-Earth Earth System model to conduct a series of targeted simulations aimed at enhancing our understanding of the role of atmospheric organic aerosol parameterizations through the implementation of high-precision chemistry and emission modeling schemes. Within this framework, targeted developments have been made to the model's atmospheric composition parameterizations, particularly concerning the primary and secondary sources of atmospheric aerosols. The aim of this project was to improve the representation of fine and coarse organic atmospheric aerosols in the EC-Earth AerChemMIP model configuration, with the overarching objectives being:

- To implement state-of-the-art parameterizations for secondary organic aerosol (SOA) formation.
- To integrate the main bioaerosol species (including bacteria, fungal spores, and pollen grains), simulated based on ecological and meteorological factors.

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Summary of problems encountered

(If you encountered any problems of a more technical nature, please describe them here.)

Experience with the Special Project framework

(Please let us know about your experience with administrative aspects like the application procedure, progress reporting etc.)

This Special Project was essential for the planned developments within the EC-Earth framework, as it exclusively relies on HPC infrastructures. Utilizing, on the other hand, alternative infrastructures would significantly impede timely objective achievement and necessitate additional resources, e.g., approximately 400-500 cores optimal for a complete Earth System Model (ESM) simulation. Furthermore, the memory demands for ESM simulations are substantial; i.e., depending on the desired output, the atmosphere-chemistry-land-ocean configuration may require a full node allocation to XIOS. This underscores the necessity of running models such as EC-Earth on high-performance computing (HPC) platforms like H2020, which enable realistic runtimes and facilitate the timely production of scientific results, thereby advancing the project's scientific objectives.

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Summary of results

(This section should comprise up to 10 pages, reflecting the complexity and duration of the project, and can be replaced by a short summary plus an existing scientific report on the project.)

Short summary:

Organic compounds significantly influence tropospheric aerosol mass and Earth's radiative balance. Accurate representation of organic aerosols (OA) in Earth system models (ESMs) is crucial for understanding aerosol-climate feedback. Secondary OA (SOA), formed from volatile organic compound (VOC) oxidation, involves complex processes that introduce uncertainties in fine particulate matter simulations. Additionally, inadequate representation of biological material can also lead to a severe underestimation of coarse OA mass in ESMs.

To improve organic atmospheric aerosol representation in the EC-Earth AerChemMIP model (EC-Earth3-AerChem), this project aims to:

1. Implement advanced parameterizations for SOA formation, focusing on semivolatile and intermediate-volatility organic compounds.
2. Integrate key bioaerosol types based on ecological and meteorological factors.

An updated emission framework, incorporating volatility coverage of primary organic aerosol (POA) inventories and atmospheric biological material sources, has been integrated into EC-Earth3-AerChem for this project. SOA formation from semivolatile organic compounds (SVOCs) and intermediate-volatility organic compounds (IVOCs) has been included using the ORACLE-lite module, alongside the existing biogenic SOA formation scheme from isoprene and monoterpenes. Additionally, bacteria, fungal spores, and pollen grains have been implemented here through interactive bioaerosol schemes dependent on ecosystem types, online leaf area index (LAI), and meteorological parameters from IFS. Together these developments improve both the fine and coarse organic aerosol representation within EC-Earth.

This new aerosol scheme, developed within this project, increases surface OA concentrations compared to the CMIP6 configuration, with fine OA mass primarily from IVOC emissions and coarse OA mainly comprising bioaerosols. Evaluation shows the model effectively captures absolute organic mass concentrations and seasonal variations. This work provides an initial assessment toward bridging the gap between model simulations and organic mass observations, improving understanding of OA's radiative impacts and aerosol-climate feedback in EC-Earth.

Results:

EC-Earth is a global Earth System Model (ESM) that incorporates the ECMWF Integrated Forecast System (IFS) and the Nucleus for European Modelling of the Ocean (NEMO) as its core components. EC-Earth employs the TM5-MP chemistry-transport model to simulate global tropospheric composition (van Noije et al., 2014), utilizing the KPP-based Carbon Bond Mechanism 5 (Williams et al., 2013; Myriokefalitakis et al., 2020). For this study, anthropogenic and biomass burning emissions were applied according to CMIP6 recommendations. Mineral dust is calculated online (Tegen et al., 2002), driven by meteorological parameters (van Noije et al., 2021), while biogenic emissions are sourced from the MEGAN-MACC dataset (Sindelarova et al., 2014). EC-Earth utilizes the LPJ-GUESS dynamic global vegetation model to deliver vegetation composition and distribution as the terrestrial ESM component for the carbon cycle. Note, that for the first time, LPJ-GUESS was coupled online for this project to TM5-MP via OASIS to provide LAI data every 24 hours.

Organic Aerosol Developments

A lite version of the well-documented aerosol module ORACLE v1.0 (Tsimpidi et al., 2026) has been coupled to EC-Earth3-AerChem. ORACLE-lite allows for relatively low computing resource consumption while calculating the partitioning and chemical evolution of primary organic aerosol (POA) vapors and their changes in volatility, utilizing the volatility basis set (VBS) approach. Primary organic aerosols are assumed to be emitted as either semi-volatile organic compounds (SVOCs; ~40%) or intermediate volatile organic compounds (IVOCs; ~60%): LVOCs (7.4-7.6 Tg yr^{-1}), SVOCs (31.4-31.8 Tg yr^{-1}), and IVOCs (52.8-53.1 Tg yr^{-1}), see Fig. 1.

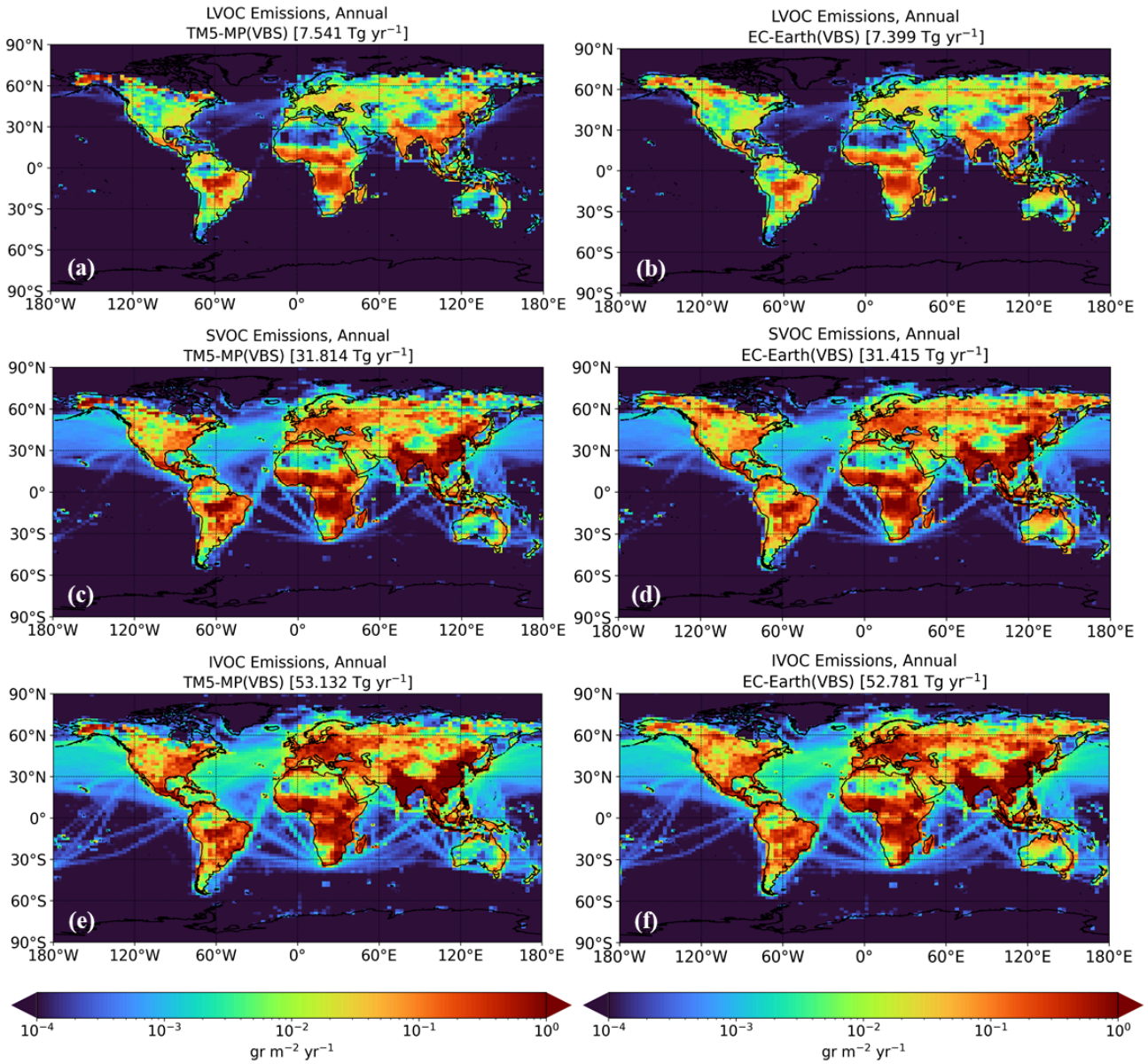


Figure 1. Annual emissions (in g m−2 yr−1) applied in the simulations of the standalone chemistry-transport model TM5-MP during 2005 (left column) and EC-Earth during 2000–2010 (right column) for: (a, b) low volatile organic compounds (LVOCs), (c, d) semi-volatile organic compounds (SVOCs), and (e, f) intermediate volatile organic compounds (IVOCs).

Figure 2 shows the annual mean surface concentrations of POA and SOA in the EC-Earth simulation with the VBS configuration for 2000–2010. Note that aerosol size distributions for POAs from SVOCs and IVOCs, as well as semi-volatile secondary organic aerosols (sv-SOA) and intermediate volatile secondary organic aerosols (iv-SOA), were determined based on M7 calculations that redistribute changes in organic aerosol (OA) mass per mode. Consequently, the new SVOC and IVOC aerosol masses for POAs and SOAs correspond to the soluble Aitken (AIS), accumulation (ACS), and coarse (COS) aerosol modes in the model. SOA concentrations remain higher than POA with increasing altitude because organic gases are efficiently transported upward, oxidized, and produce lower-volatility SOA.

EC-Earth predicts high total OA concentrations (up to 4-5 µg m^{-3}) in South America, Africa, India, and China due to higher production of SOA-iv. The oxidation of IVOCs, which produces lower-volatility products, also contributes to SOA-sv formation. In ORACLE-lite, the volatility bin representing SOA-sv corresponds to a C^* value of 10^{-2} µg m^{-3}, indicating low volatility and a predominant presence in the particle phase. Higher SOA-sv concentrations are predicted during summer compared to winter due to higher summer temperatures promoting POA evaporation and increased sunlight, which enhances subsequent photooxidation and SOA formation.

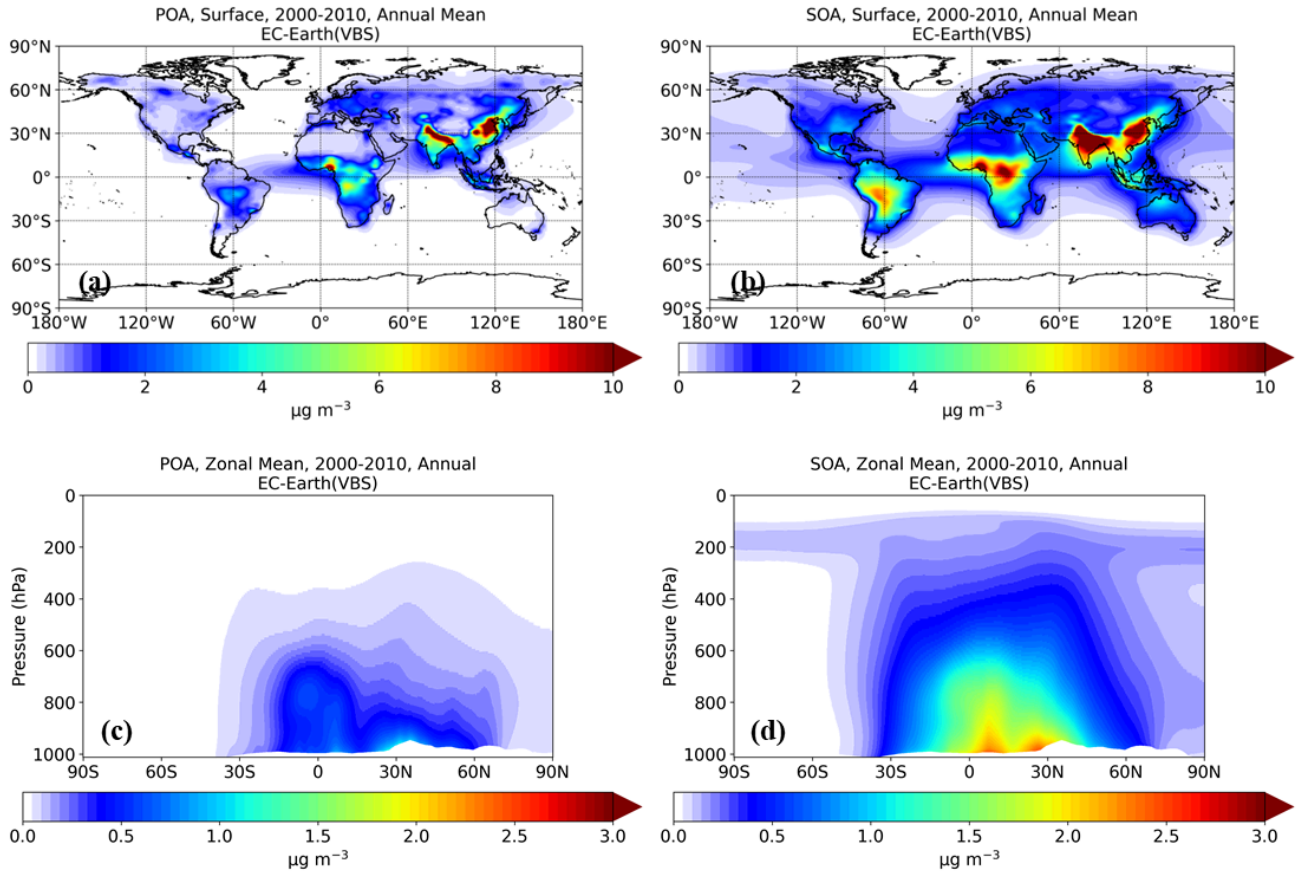


Figure 2. Annual mean concentrations of POA and SOA (in µg m−3): (a, b) surface concentrations, and (c, d) zonal values as simulated using the VBS configuration of EC-Earth during 2000–2010.

Higher annual mean concentrations of SOA-iv compared to SOA-sv are predicted, primarily due to higher emissions of IVOCs (Fig. 1) and the different formation mechanism. IVOCs can directly undergo oxidation by hydroxyl radicals, producing lower-volatility products that subsequently condense into the particle phase. Predicted SOA-iv concentrations are higher in winter than in summer, particularly in China, India, Bangladesh, and Europe. This is attributed to increased biomass burning emissions and lower temperatures, which enhance partitioning of semi-volatile OA components into the particle phase. However, in regions such as South America and southern Africa, where major rainforests like the Amazon and Congo Basin are located, SOA-iv concentrations are higher during summer due to wildfires.

Figure 3 compares predicted PM2.5 OA concentrations from TM5-MP and EC-Earth simulations with measurements in 2005. Each point represents a monthly average at a monitoring station. The VBS configuration of TM5-MP predicts higher OA concentrations than the default, with results generally closer to the 1:1 line. Both TM5-MP simulations underpredict OA concentrations, as shown by negative MB and NMB values; the VBS configuration reduces this underprediction by approximately half (MB = −0.28 µg m−3, NMB = −13.2 %) compared to the default (MB = −0.57 µg m−3, NMB = −27.1 %). NME and RMSE values, already low in the default simulation (NME = 42 %, RMSE = 1.57 µg m^{-3}), further improve in the VBS simulation (NME = 38.9 %, RMSE = 1.5 µg m^{-3}), indicating reduced scatter.

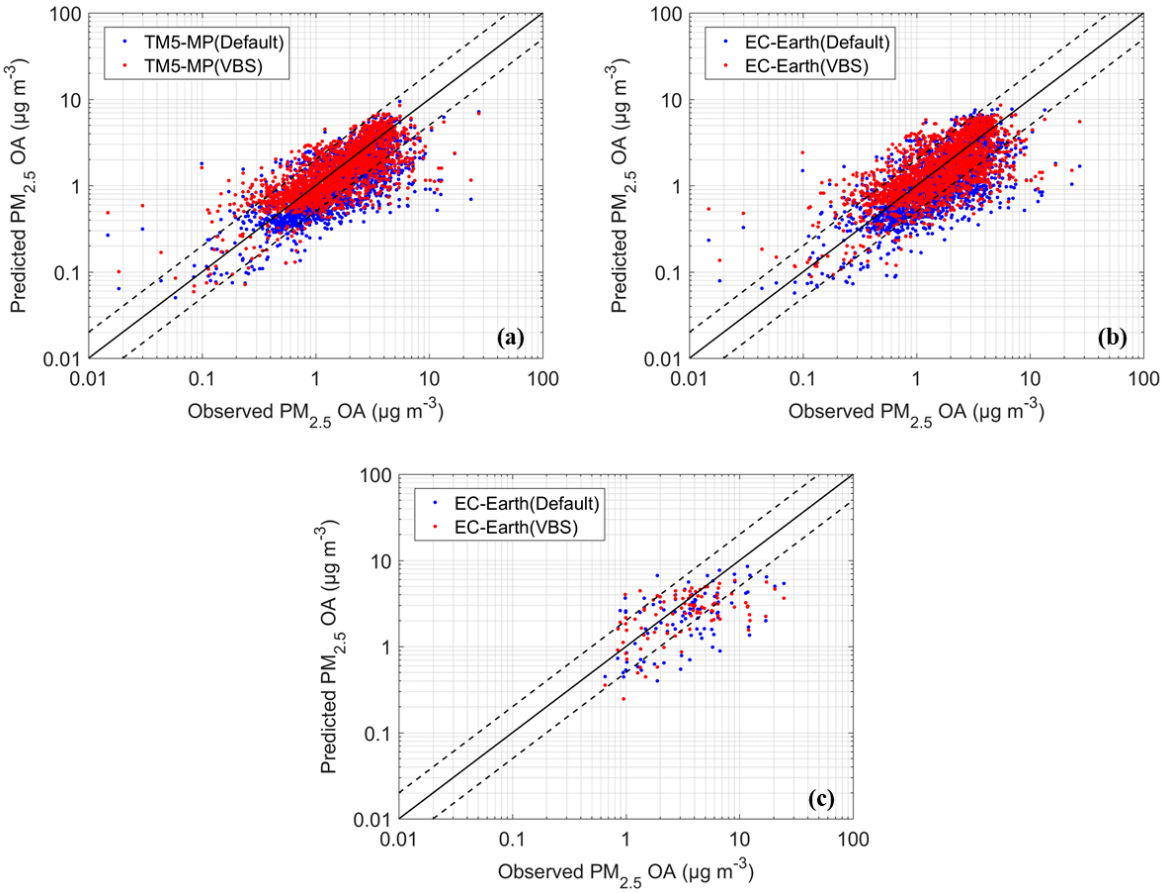


Figure 3. Organic mass concentrations from simulations of: (a) TM5-MP during 2005, (b) EC-Earth during 2005, and (c) EC-Earth during 2010. Scatterplots of the first row compare predicted PM2.5 OA concentrations (in µg m−3) with observations from both the IMPROVE and EMEP monitoring networks, while the second row shows a single comparison only with EMEP. Models' results are shown for the default configuration (blue) and the VBS configuration (red). Each point represents a monthly average value at a monitoring site.

Bioaerosol Developments

Bacteria (BCT) emissions are parameterized using near-surface observations and model estimations to establish optimal BCT flux rates for monodisperse spherical particles with a geometric mean diameter of 1 µm across all ecosystems, as outlined in Burrows et al. (2009). Fungal spore (FNG) emission fluxes, with an assumed geometric mean diameter of 3 µm, are linearly dependent on the LAI (calculated by LPJ-GUESS) and specific humidity (calculated by IFS), following parameterizations by Hummel et al. (2015) and Heald and Spracklen (2009).

Pollen grains (PLN) are modeled in EC-Earth as a lumped tracer for particles with diameters ranging from 10 to 125 μm (Hoose et al., 2010; Jacobson and Streets, 2009; Myriokefalitakis et al., 2017). EC-Earth treats pollen as an insoluble aerosol with a density of 800 kg m^{-3} and an average diameter of 22 μm, specifically representing birch pollen (Kouznetsov and Sofiev, 2012). A pollen flux (f_{PLN}) of 0.5 m^{-2} s^{-1} is assumed, based on a parameterization by Jacobson and Streets (2009), and is linearly dependent on the LPJ-GUESS' LAI values.
Following Sofiev et al. (2013), corrections based on short-term meteorological conditions are applied to this dynamic release rate, specifically using correction functions dependent on wind speed, relative humidity, and precipitation rate. Corrections related to precipitation and humidity are derived from known "prohibiting" thresholds that completely suppress pollen release. Until these thresholds are reached, these variables neither affect nor promote pollen release. The lower and upper thresholds of relative humidity are set at q_{low} = 50% and q_{high} = 80% (Sofiev et al., 2013). Near these thresholds, a linearly decreasing transition function is employed. For precipitation, P_{low} = 0 indicates that any significant rain suppresses pollen release and scavenges emitted grains. High relative humidity associated with rain can also halt pollen release, affecting areas larger than the rain event itself. We consider a threshold of P_{high} = 0.5 mm hr^{-1} as the grid cell average rate that completely suppresses pollen emission. Additionally, in low wind conditions with developed thermal convection, turbulence alone can initiate release by generating sub-grid convective winds. Stronger winds facilitate the release from open catkins, but after a certain wind speed is reached, further increases do not affect the release rate, which becomes limited by the availability of pollen grains ready to fly from the catkins. Assuming U_{satur} = 5 m sec^{-1}, $f_{stagnant}$ = 0.5, and $f_{promote}$ = 1, we conclude that wind speeds of approximately 1 m s^{-1} have no impact, while very strong winds can lead to a threefold increase in release compared to calm conditions, Finally, the assumed thresholds for the start and the end of pollen release account for the cut-off temperature $T_{c\text{-}o}$ = 3.5°C with the start season at D = 60 (i.e., March 1 for the Northern Hemisphere).

Table 1. The modal structure of M7 with its aerosol components: sulphate (SO4), black carbon (BC), primary organic matter (POM), secondary organic aerosols (SOA), sea salt (SS), mineral dust (DU), and primary bioaerosol particles (PBAP). The range of aerosol particle radius (r) in the respective mode is given in μm.

Modes	Radius range (μm)	mixed/soluble	insoluble
Nucleation	$r \leq 0.005$	SO4, SOA	
Aitken	$0.005 < r \leq 0.05$	SO4, BC, POM, SOA, SS, DU	BC, POM, SOA
Accumulation	$0.05 < r \leq 0.5$	SO4, BC, POM, SOA, SS, DU, PBAP	DU, PBAP
Coarse	$r \leq 1$	SO4, BC, POM, SOA, SS, DU, PBAP	DU, PBAP

For the first time to our knowledge, the M7 module has been extended by adding insoluble and soluble/mixed bioaerosols (PBAP) as new aerosol component (see Table 1) that correspond to the sum of the respective bioaerosols in the model (bacteria, fungal spores and pollen). To account for the processes affecting these new bioaerosol insoluble species (i.e., coagulation and condensation), intramodal coagulation is assumed to occur, allowing the new accumulation and coarse insoluble modes to also contain bioaerosols in addition to dust. It is assumed, however, that the sticking coefficient for bioaerosol species is small enough to prevent coagulation among them. Conversely, when an insoluble bioparticle has enough soluble material associated with it, it is allowed to move to the mixed modes and is defined as "aged." The aging of insoluble bioparticles is assumed to result from the condensation of sulfuric acid and exist then in M7 as internally mixed aerosols

Overall, our calculations indicate that EC-Earth estimates a total global annual flux of bioaerosols at approximately 84 Tg yr^{-1}, with a global mean lifetime of about 1.4 days; applying a mean OM:OC mass ratio of 2.6, these emissions correspond to ~32 Tg C yr^{-1}.

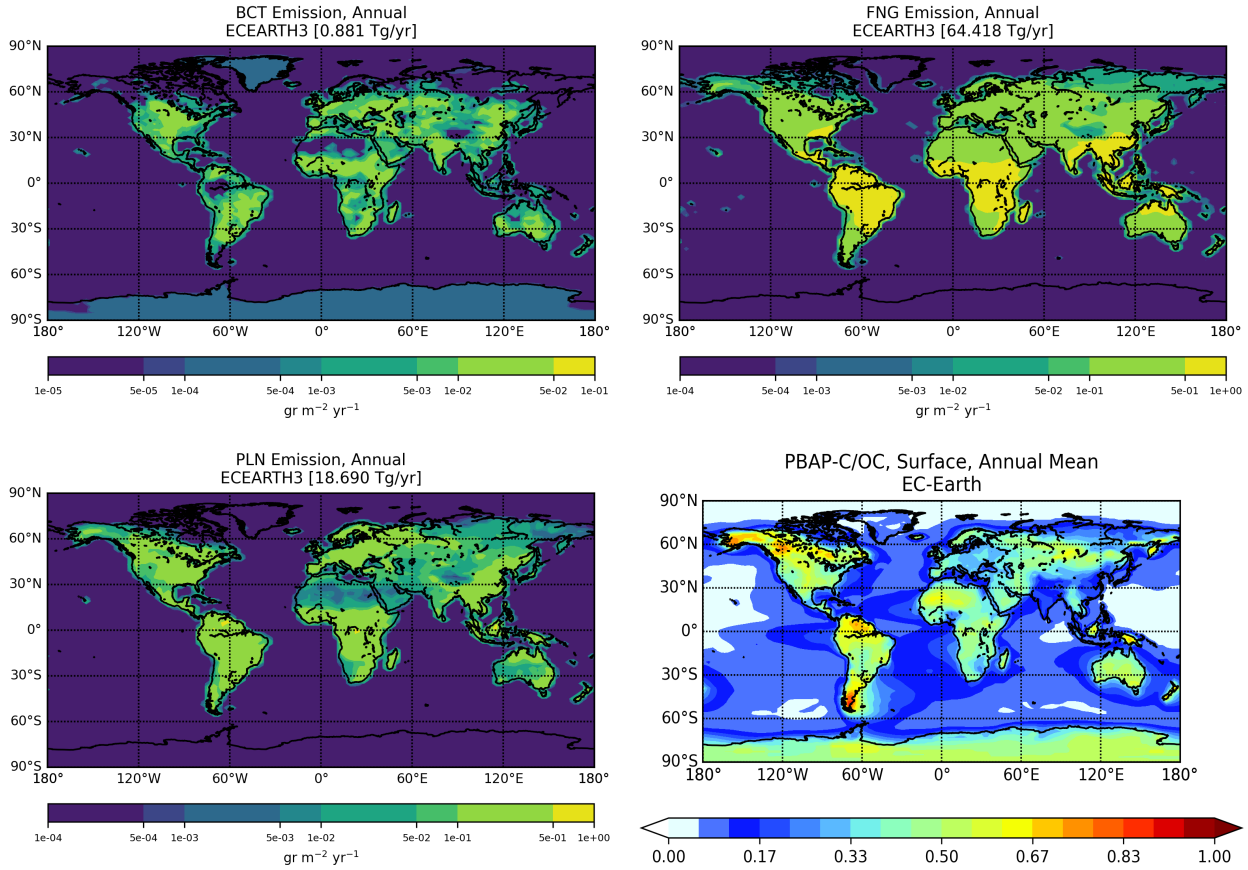
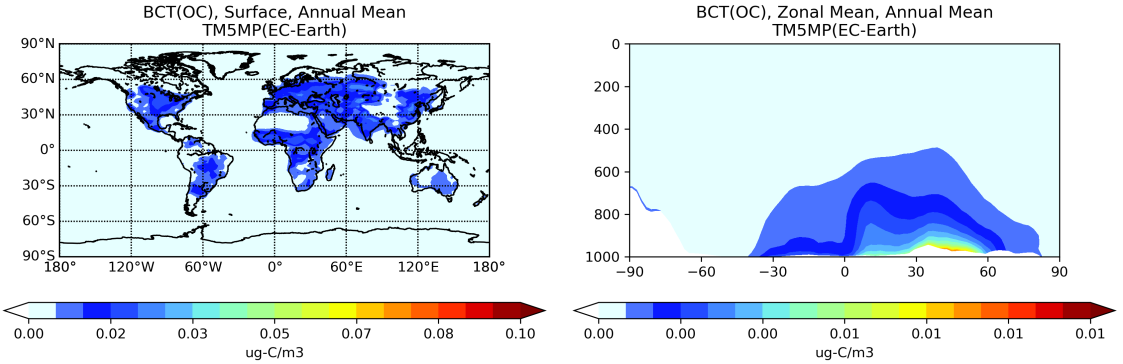


Figure 4. Present day calculated emission rates (gr m-2 yr-1) for bacteria (BCT), fungal spores (FNG) and pollen grains (PLN) along with the contribution of bioaerosols (PBAPs) to the surface organic carbon concentrations in EC-Earth.

A thorough assessment of present-day atmospheric bioaerosol concentrations, along with a detailed comparison with prior model estimates available in the literature is presented in this technical report. Figure 4 depicts the simulated surface and zonal mean bioaerosol concentrations calculated by EC-Earth for bacteria, fungi, and pollen. For this analysis, the organic matter to organic carbon ratio (OM:OC) for all bioaerosols is assumed to be 2.6, using the molecular weight of mannitol (31 g mol^{-1}) (Heald and Spracklen, 2009) as a universal biotracer for all bioaerosol types in the model. Notably, hydrophilic aerosols exhibit faster removal from the troposphere through dry and wet deposition compared to hydrophobic aerosols.



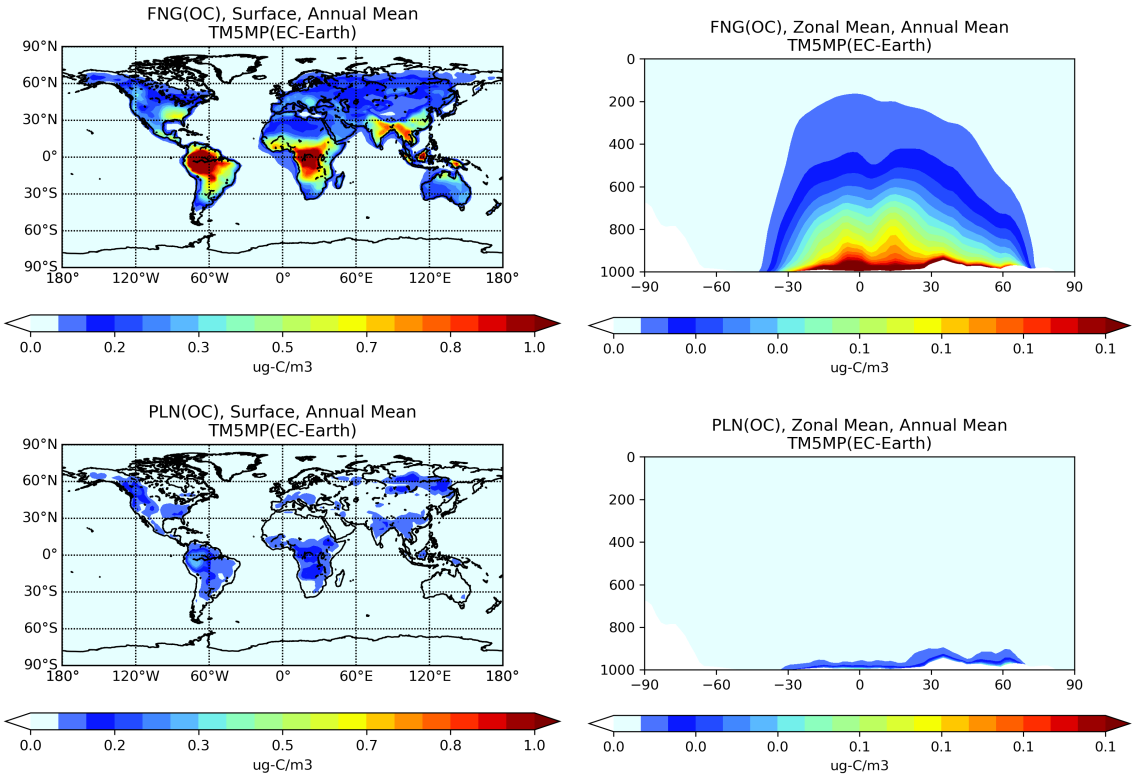


Figure 5. Surface (left) and zonal mean (right) mass concentrations of the bioaerosol aerosols (µg-C m-3), as simulated for the present day by the atmospheric component of EC-Earth (TM5-MP) for bacteria (top), fungal spores (middle), and pollen grains (bottom).

EC-Earth simulations indicate elevated surface FNG mass concentrations across most regions relative to the other bioaerosol types (BCT and PLN) within the model domain (Fig. 5). Maximum surface FNG concentrations occur in the Southern Hemisphere, particularly over the tropical forests of South America (Amazon Basin), the savannas of Africa (Congo Basin), and Southern Asia, which can be attributed to dense vegetation cover. In contrast, the Northern Hemisphere exhibits lower surface concentrations due to sparse vegetation and a predominance of urbanization. Overall, the calculated global burdens for the present day indicate that the majority of the total simulated bioaerosol mass (579 Gg) exists in the atmosphere as FNG (~93%), followed by BCT (~4%), while PLN comprises approximately 3% in the model due to its short lifetime (~ 0.1 days) owing to its rather large size (supercoarse aerosol mode).

Figure 6 compares calculated monthly mean pollen and fungal spore concentrations from the bioaerosol model configuration with observational data from the Hyytiälä Forest Station, University of Helsinki (Manninen et al., 2014) and (Schumacher et al., 2013). The model accurately represents both absolute concentrations and seasonal variations of these bioaerosol types. It is important to note that fungal spores are treated identically to FBAP within the model. Additionally, the enhanced derived OA concentrations from this new configuration are expected to positively impact the simulated aerosol optical depth of EC-Earth, particularly in the coarse aerosol mode.

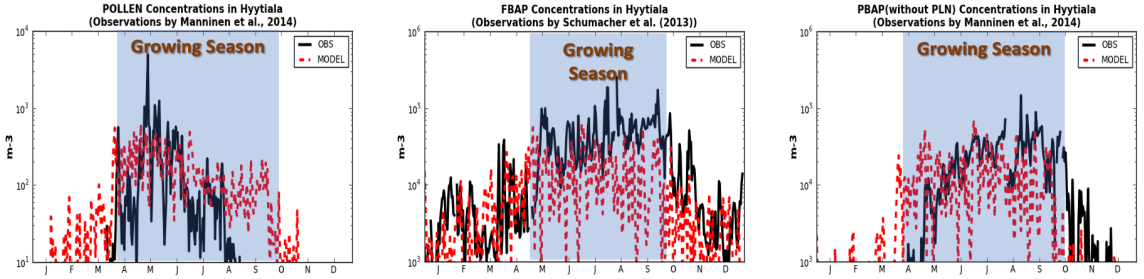


Figure 6. Comparison of calculated monthly mean pollen and fungal spore surface number concentrations (# m^{-3}) for present-day EC-Earth model simulation (red dashed lines) against observations collected in the Hyytiälä Forest Station of University of Helsinki from [(Manninen et al., 2014)] and [(Schumacher et al., 2013)] (black lines).

This project further aimed to estimate the pre-industrial (PI; 1851-1860), present-day (PD; 2001-2010), and future (2090-2100) climate impacts on bioaerosol concentrations. We also examined their feedback using time-slice global simulations with the EC-Earth3-AerChem Earth System Model (ESM). Utilizing our novel model capabilities, we estimated bioaerosol concentrations and assessed their impact on the global organic carbon (OC) burden. Additionally, we quantified the contributions of meteorology and vegetation composition for PI, PD, and future scenarios following the Shared Socioeconomic Pathways (SSPs) of CMIP6 (Eyring et al., 2016). Although our primary focus is on bioaerosol cycles and their drivers, the assessment of LAI in future scenarios has been understudied, with implications beyond the bioaerosol cycle. Initial conditions for atmospheric tracers, gas-phase species, and aerosols are established using one year of spin-up to ensure realistic global-scale concentrations; the second year of simulation is utilized for the analyses. Simulations are run with IFS, LPJ-Guess, and TM5-MP coupled, neglecting potential feedback between the atmosphere and the ocean to maintain consistent conditions.

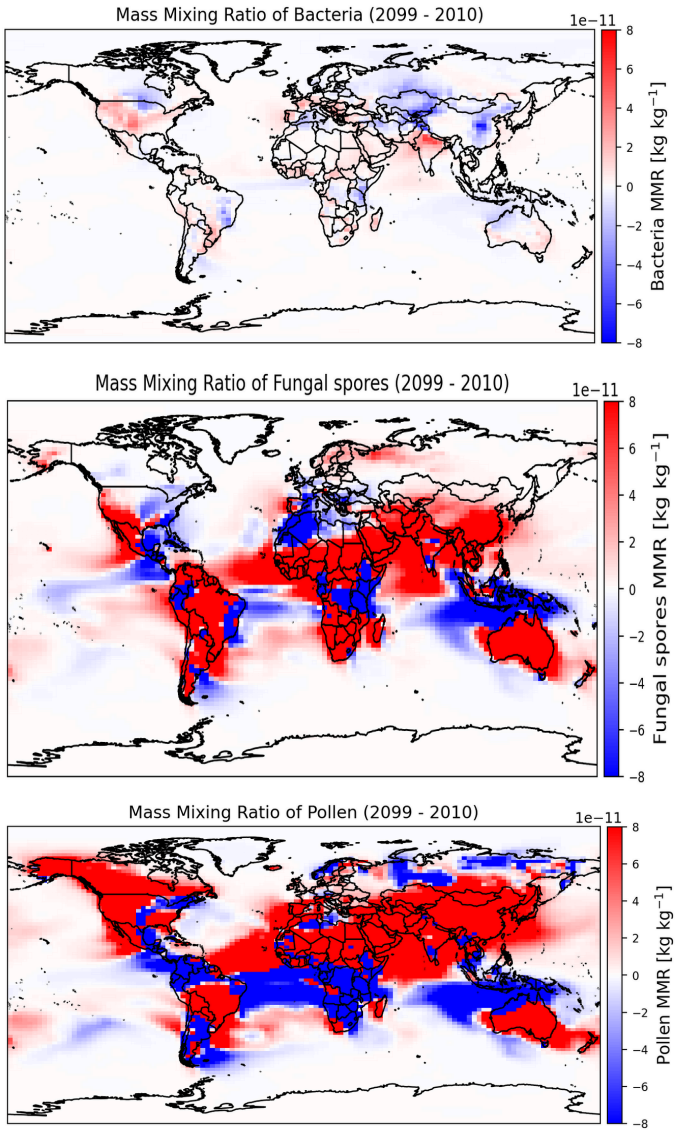


Figure 7. Bacteria (top), Fungal spores (middle), and Pollen grain concentrations (bottom) absolute difference for present-day and future simulation as calculated by EC-Earth.

Figure 7 illustrates that future bioaerosol responses are driven by increased LAI at mid- and high latitudes and localized vegetation declines in parts of the tropics. Atmospheric bacterial concentrations primarily respond to large-scale changes in precipitation, transport, and wet removal, resulting in enhanced burdens over drier continental regions and decreases in wetter tropical and monsoon-influenced areas. Fungal spore emissions and concentrations closely track vegetation

changes, showing widespread increases over vegetated mid- and high-latitude regions and localized declines in the tropics linked to heat and moisture stress. Pollen grains exhibit the most complex response, reflecting the combined effects of LAI changes and short-term meteorological controls on release, including wind speed, humidity, and precipitation. All in all, future bioaerosol distributions are shaped by distinct yet interacting climate-driven mechanisms, ranging from vegetation restructuring to altered precipitation and atmospheric transport, leading to pronounced regional contrasts by the end of the century. Moreover, the new scheme results in increased surface OA concentrations compared to the CMIP6 model configuration, with the coarse organic aerosol fraction predominantly consisting of atmospheric biological material sources.
Overall, this Special Project successfully delivered two major developments within EC-Earth3 ESM: an advanced SOA representation based on ORACLE-lite and a fully interactive bioaerosol framework. Together these developments substantially improve the representation of both fine and coarse organic aerosols while maintaining computational efficiency suitable for ESM applications.

List of publications/reports from the project with complete references

1. **Myriokefalitakis, S.**, Kakavas, S., Chatziparaschos, M., Karydis, V., Tsimpidi, A., Karathanasopoulos, O., Nieradzik, L., Kanakidou, M., and Pandis, S. N.: *An Improved Representation of Organic Aerosol Composition and Atmospheric Evolution in the EC-Earth3-AerChem model*, EGU 2025, https://doi.org/10.5194/egusphere-egu25-11354, 2025.
2. Kakavas, S., **Myriokefalitakis, S.,** Tsimpidi, A. P., Karydis, V. A., and Pandis, S. N.: *Implementation of the ORACLE (v1.0) organic aerosol composition and evolution module into the EC-Earth3-AerChem model,* Geoscientific Model Development, 19, 4271–4288, https://doi.org/10.5194/gmd-19-4271-2026, 2026.

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Future plans

(Please let us know of any imminent plans regarding a continuation of this research activity, in particular if they are linked to another/new Special Project.)

Our initial work was kindly extended for an additional year (until June 2026), and our research activity focused on finalizing our publications and EGU presentations. We have completed one publication on GMD that was based on the proposed model developments, focusing in particular on SOA, and one more is ready to be submitted, focusing on bioaerosol developments.

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