SPECIAL PROJECT PROGRESS REPORT

All the following mandatory information needs to be provided. The length should *reflect the complexity and duration* of the project.

Reporting year	2025
Project Title:	EC-Earth Atmospheric Composition developments
Computer Project Account:	spgrmyri
Principal Investigator(s):	Stelios Myriokefalitakis
Affiliation:	National Observatory of Athens (NOA)
Name of ECMWF scientist(s) collaborating to the project (if applicable)	…… … …… …
Start date of the project:	07/11/2024
Expected end date:	31/12/2026

Computer resources allocated/used for the current year and the previous one

(if applicable)

Please answer for all project resources

		Previous year		Current year	
		Allocated	Used	Allocated	Used
High Performance Computing Facility	(units)	3,800,000	269,306	3,800,000	3,101,069
Data storage capacity	(Gbytes)	-	-	-	-

Summary of project objectives (10 lines max)

During this project, the EC-Earth Earth System model (ESM) was used to conduct a series of 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 organic aerosols. Overall, the aim of the first year of the 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 principal bioaerosol types (including bacteria, fungal spores, and pollen grains), simulated based on ecological and meteorological factors.

Summary of problems encountered (10 lines max)

The proposal was submitted in January 2024 with a two-year duration. However, due to difficulties with the local representative, the special project did not begin until November 2024.

Summary of plans for the continuation of the project (10 lines max)

The main developments of the model have already been completed, and results are now being prepared for the final publications. The latter indicates that it is necessary to extend the duration of this special project up to 31/12/2026.

List of publications/reports from the project with complete references

- **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.

Summary of results

If submitted **during the first project year**, please summarise the results achieved during the period from the project start to June of the current year. A few paragraphs might be sufficient. If submitted **during the second project year**, this summary should be more detailed and cover the period from the project start. The length, at most 8 pages, should reflect the complexity of the project. Alternatively, it could be replaced by a short summary plus an existing scientific report on the project attached to this document. If submitted **during the third project year**, please summarise the results achieved during the period from July of the previous year to June of the current year. A few paragraphs might be sufficient.

Organic compounds play a significant role in the total tropospheric aerosol mass and affect Earth's radiative balance both directly and indirectly. This highlights the need for an accurate representation of organic aerosols (OA) in Earth system models (ESMs) to improve our understanding of aerosol-climate feedback. Secondary OA (SOA), which is formed from the oxidation of volatile organic compounds (VOCs), involves complex processes that can introduce uncertainties in model simulations of fine particulate matter. Additionally, the biological material emitted into the atmosphere is often inadequately represented in most models, resulting in an underestimation of coarse OA mass in ESMs. To enhance the representation of the organic atmospheric aerosols in the EC-Earth AerChemMIP model configuration (EC-Earth3-AerChem), this project aims:

1. to implement advanced parameterizations for SOA formation, focusing on the roles of semivolatile and intermediate-volatility organic compounds, as well as
2. to integrate key types of bioaerosols based on ecological and meteorological factors.

A new emission framework has been integrated into the EC-Earth3-AerChem model, which utilizes the volatility coverage of primary organic aerosol (POA) inventories and sources of atmospheric biological material. 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. The model's chemical oxidation of organic vapors has also been added to the model's chemical solver. Additionally, the three primary types of bioaerosols—bacteria, fungal spores, and pollen grains—have been implemented through interactive bioaerosol schemes that are dependent on ecosystem types and real-time calculations of leaf area index (LAI) provided by LPJ-GUESS, along with meteorological parameters from IFS. In the model, bioaerosols are emitted as insoluble particles but can transition to the soluble aerosol mode due to atmospheric aging processes. The size distribution of these new species is calculated using the M7 aerosol microphysics module. This new scheme results in increased surface OA concentrations compared to the CMIP6 model configuration, with fine organic aerosol mass primarily derived from IVOC emissions and the coarse organic aerosol fraction mainly comprising bioaerosols. Evaluation of the results indicates that the model effectively captures absolute organic mass concentrations and seasonal variations. The enhanced OA concentrations are expected to positively influence the simulated aerosol optical depth in EC-Earth. Overall, this work provides an initial assessment toward bridging the gap between model simulations and organic mass observations, thereby improving our understanding of OA's radiative impacts and the aerosol-climate feedback mechanism in EC-Earth.

For the secondary organic aerosol (SOA) calculations, a lite version of the well-documented aerosol module ORACLE (Tsimpidi et al., 2014) 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%). Then, the equilibrium model determines 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), based on M7 calculations that redistribute changes in organic aerosol (OA) mass per mode.

OA component	Burden (Tg)
POA	*0.013*
SOA-sv	*0.537*
SOA-iv	*1.389*
bSOA-v	*0.994*

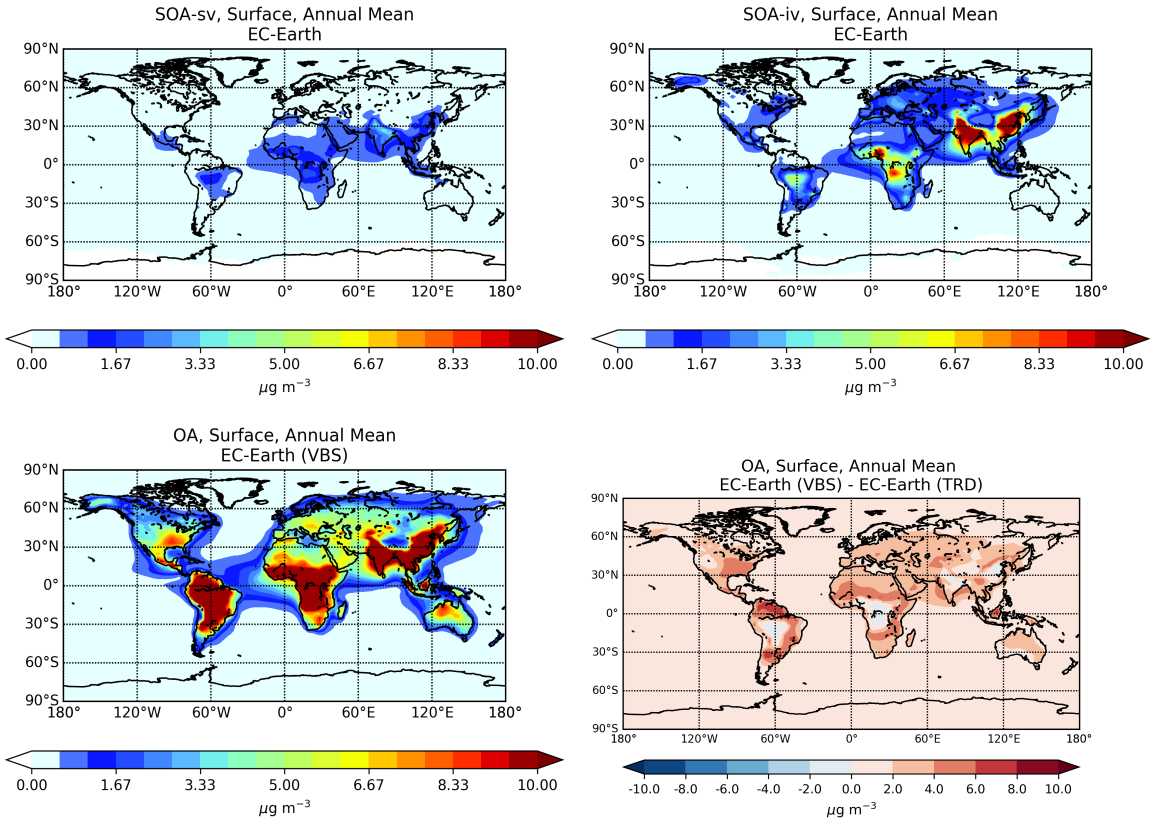
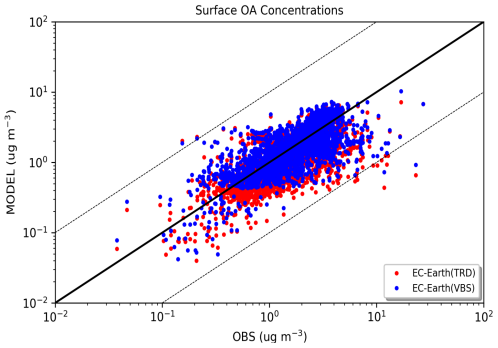


Figure 1. Annual mean surface concentrations (μg m^{-3}) with the new OA configuration (VBS) for a) SOA-sv, b) SOA-iv, c) total OA, along with d) the respective difference compared to the original model configuration with traditional organic aerosol representation (TRD).

Our results indicate that the new model configuration leads to higher surface OA concentrations across most regions compared to the traditional (TRD) OA configuration of EC-Earth3-AerChem. Specifically, the calculated global average surface OA concentration is approximately 1.15 μg m^{-3}, which is about 29% higher than the traditional OA configuration. The most significant increases (>50%) in surface OA concentrations occur in the Northern Hemisphere, particularly downwind of Southern Asia and at the outflow of the Pacific and Atlantic Oceans, due to the photochemical aging of anthropogenic IVOCs and SVOCs and their efficient transport away from the sources. In contrast, only slight decreases (<10%) in surface concentrations are observed over the tropical forests of South America (Amazon Basin) and the savannas of Africa (Congo Basin), where OA is predominantly of biomass burning and biogenic origin.



- **EC-Earth(TRD): N=2105, R=0.504, NMB=-12.266, RSME=1.612 µg m^{-3}, NME=44.965 µg m^{-3}**
- **EC-Earth(VBS): N=2105, R=0.515, NMB=8.703, RSME=1.548 µg m^{-3}, NME=42.476 µg m^{-3}**

Figure 2. Comparison of calculated monthly mean OA surface concentrations (µg m-3) for the standard EC-Earth configuration with a traditional description of POA emissions (TRD) and the new VBS scheme with monthly mean observations (Tsimpidi et al., 2014) as compiled from: the European Monitoring and Evaluation Programme (EMEP; http://nilu.no/projects/ccc/onlinedata/pm/), the Interagency Monitoring of protected Visual Environments(IMPROVE; http://vista.cira.colostate.edu/improve/Data/IMPROVE/improve_data.htm, short-term measurement data collected over East Asia (Jo et al., 2013).

For bioaerosol calculations, bacteria (BCT) emissions are parameterized as outlined in Burrows et al. (2009), 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. Fungal spore (FNG) emission fluxes are treated as linearly dependent on the LAI (as calculated by LPJ-GUESS) and specific humidity (as calculated by IFS), following parameterizations by Hummel et al. (2015) and Heald and Spracklen (2009), with a geometric mean diameter of 3 µm assumed. Pollen grains (PLN) are represented as an insoluble aerosol with a density of 800 kg m^{-3} and a geometric mean diameter of 22 µm, specifically reflecting birch pollen (Kouznetsov and Sofiev, 2012). A global mean pollen flux of 0.5 m^{-2} s^{-1} (Jacobson and Streets, 2009) is assumed, linearly dependent on the LAI values and adjusted for monthly and diurnal variations (Myriokefalitakis et al., 2017).

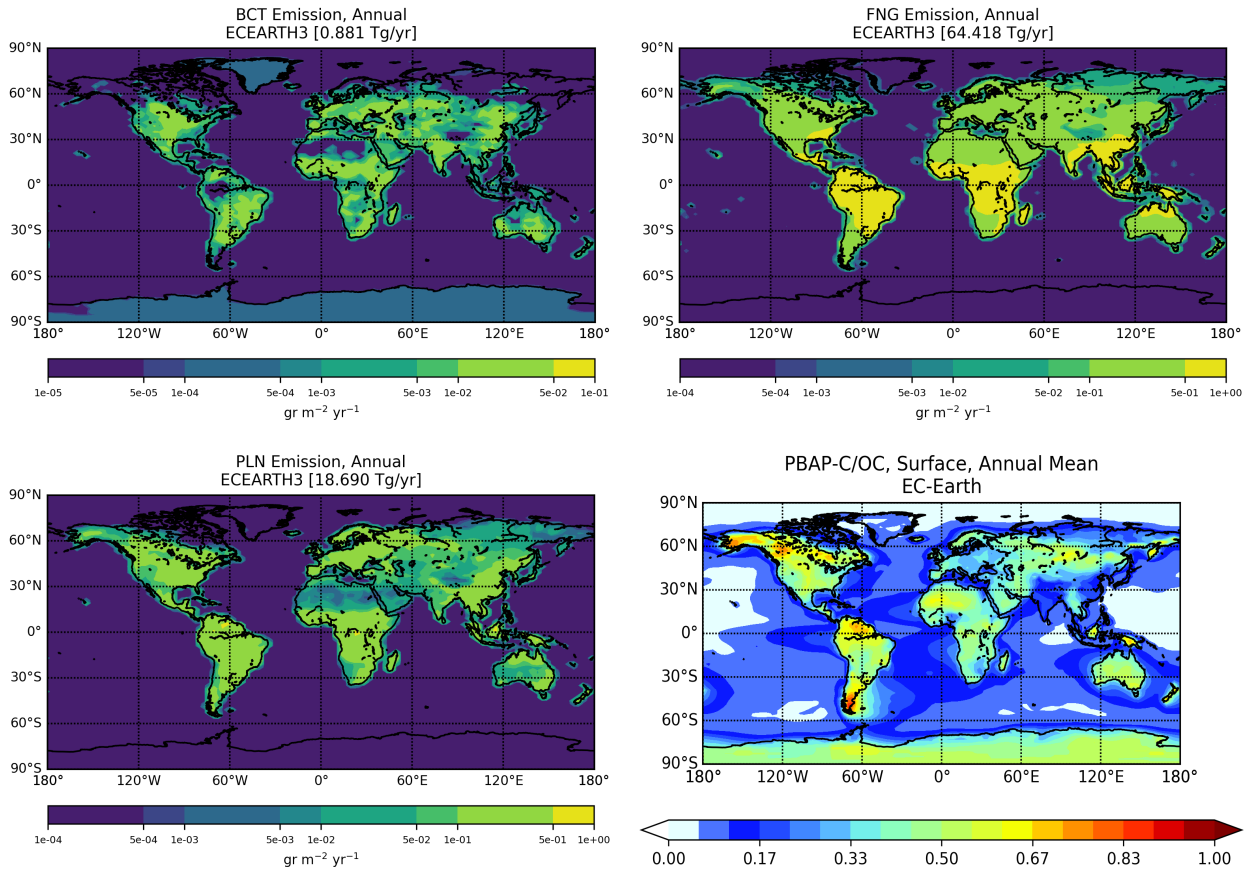


Figure 3. Present day calculated emission rates (gr m^{-2} yr^{-1}) for bacteria (BCT), fungal spores (FNG) and pollen grains (PLN) along with the contribution of bioaerosols (PBAPs) to the surface organic carbon concentrations in EC-Earth.

Additionally, for this work, the M7 microphysics module (Vignati et al., 2004) has been extended to include insoluble and soluble/mixed primary biological aerosol particles (PBAPs) as new aerosol species. 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}.

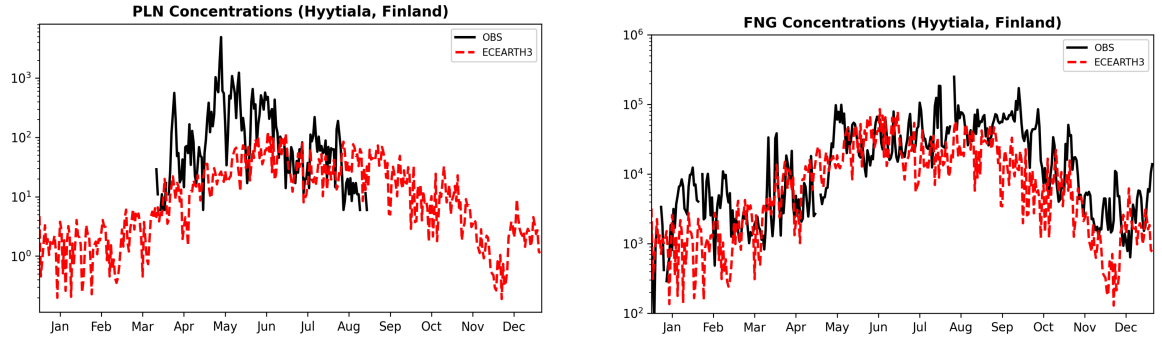


Figure 4. Comparison of the calculated daily mean surface concentrations of pollen (PLN) and fungal spores (FNG), measured in # m^{-3}, derived from the present-day EC-Earth model simulation (red dashed lines) conducted against observational data (black lines) obtained from the Hyytiälä Forest Station at the University of Helsinki (Manninen et al., 2014, Schumacher et al., 2013). Note, that for the purposes of this comparison, fungal spores (FNG) are here assumed as fluorescent biological aerosol particles (FBAPs).