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	2024
Project Title:	FLEXPART transport simulations and inverse modelling of atmospheric constituents
Computer Project Account:	spatvojt
Principal Investigator(s):	Marina Dütsch
Affiliation:	University of Vienna – Department of Meteorology and Geophysics
Name of ECMWF scientist(s) collaborating to the project (if applicable)	…………………………………………………………………… ……………………………………………………………………
Start date of the project:	2024
Expected end date:	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)			2000000	
Data storage capacity	(Gbytes)			4000	

Summary of project objectives (10 lines max)

The Lagrangian particle dispersion model FLEXPART (Stohl et al., 2005, Bakels et al., 2024) is run with ECMWF data to explore the dispersion and transport of various atmospheric constituents. The model is used with inversion techniques to enhance the knowledge about the emissions of many atmospheric compounds. This helps to get a better understanding of their impact on the Earth's climate system and air quality and to improve transport simulations of these substances. By performing domain-filling simulations the model is used to develop Lagrangian climatologies of heat and energy transport in the atmosphere and to perform case studies of extreme weather events.

Summary of problems encountered (10 lines max)

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

We will continue the analyses on our research topics (see summary of results). In addition, we plan to develop a web service, called FLEXWEB, where FLEXPART can be run in the cloud via a web interface. FLEXWEB will use ERA5 data as input for the meteorological fields and will give users worldwide access to FLEXPART without the need for installation on a local HPC system or downloading meteorological input data. A first version of the web service is already running on our local cluster (https://flexweb.wolke.img.univie.ac.at/), and our goal for the next year is to move it to a cloud service like the European Weather Cloud.

List of publications/reports from the project with complete references

Baier, K., Rubel, M., & Stohl, A. (2023). The 3-Week-Long Transport History and Deep Tropical Origin of the 2021 Extreme Heat Wave in the Pacific Northwest. *Geophysical Research Letters*, *50*(24), e2023GL105865.

Evangelou, I., Tatsii, D., Bucci, S., & Stohl, A. (2024). Atmospheric Resuspension of Microplastics from Bare Soil Regions. *Environmental Science & Technology,* 58(22), 9741-9749.

Tatsii, D, Bucci, S., Bhowmick, T., Guettler, J., Bakels, L., Bagheri, G., Stohl, A (2024). Shape Matters: Long-Range Transport of Microplastic Fibers in the Atmosphere. *Environmental Science & Technology*, 58(1), 671-682.

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.

1) Lagrangian re-analysis dataset

We created a Lagrangian re-analysis, based on the ERA5 dataset from ECMWF (Hersbach et al., 2020), on a one-hourly basis. Since last report, we extended the dataset to include all years from 1940 until the end of 2023.

In summary, we divided the full time range in 12 periods with a three month overlap. We ran our domain-filling transport model simulation with the Lagrangian particle dispersion model FLEXPART (Bakels et al., 2024), using six million particles. This dataset is suitable e.g. for establishing transport climatologies and global statistics. The aim is to publish the dataset to the scientific community by the end of this year.

We are close to submitting a paper using this dataset to study extreme events in a pristine part of the western Amazon rainforest. In this work, we investigated the role of atmospheric transport in the occurrence of extreme heat and drought events.

2) Lagrangian analysis of the 2021 extreme heat wave in the Pacific Northwest

The heat wave in late June of 2021 set new temperature records in the Pacific Northwest. In Lytton the highest temperature ever recorded in Canada was measured. We compared the atmospheric air mass transport and heating processes associated with this heat wave with the 34 other most extreme heat events in the same region during the period 1960–2021 using FLEXPART, and found significant differences in the heat waves (Figure 1). In June 2021 most of the air was coming from the Philippine Sea, with more than 40% of the air located south of 15°N, and anomalous advection of sensible and latent heat from the Tropics was the dominant cause of the heat wave. The latent heat was efficiently converted into sensible heat by precipitation, which was unique, as most other extremes experienced net diabatic cooling.

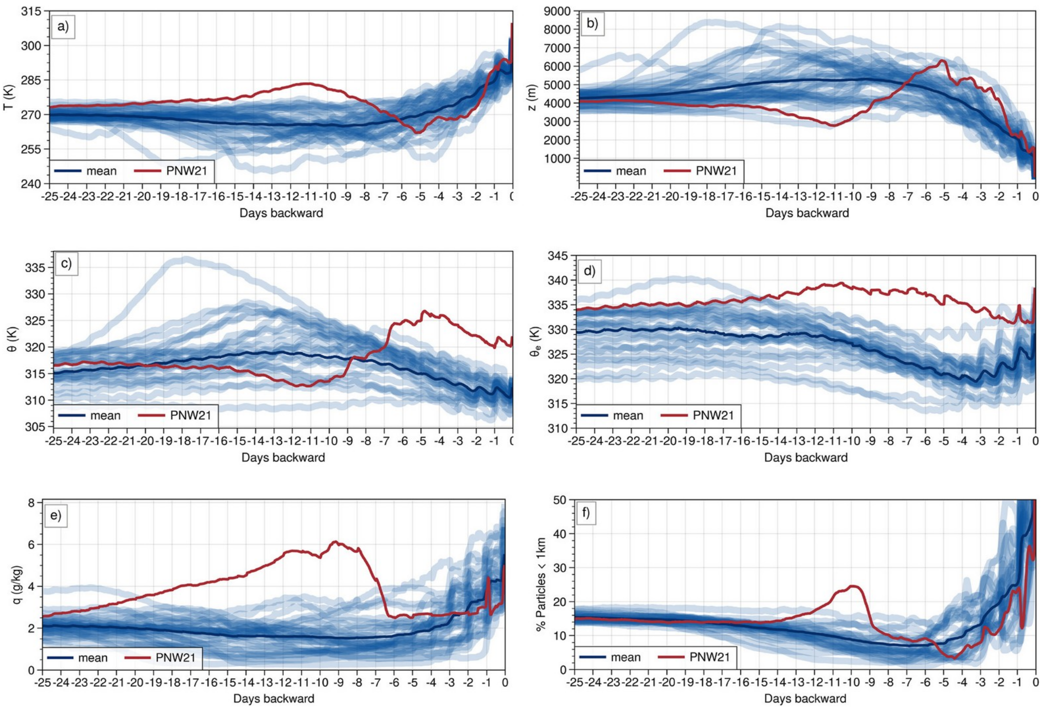

Figure 1: Meteorological parameters of the transported air as a function of time prior to arrival for all extreme events. Red solid lines represent the heat wave in June 2021 (PNW21), semitransparent thick blue lines represent each individual extreme event, and solid dark blue lines show the mean over these events, excluding PNW21. (a) Air temperature T; (b) height above sea level z; (c) potential temperature θ; (d) equivalent potential temperature θ_e; (e) specific humidity q; (f) the fraction of particles below 1 km agl.

3) Sources of methane (CH_4) in the Arctic from ship measurements

Methane is a greenhouse gas that has a global warming potential (GWP) of 28–36 times more potent than that of carbon dioxide on a 100-year timescale. In the Arctic, the average atmospheric concentration of methane is currently about 1,895 ppb (1,820 ppb is the global average). The natural Arctic methane emissions are dominated by high-latitude wetlands but with high uncertainties in the magnitude. In addition, water in the Arctic Ocean does not mix well, and the methane produced by bacteria gets preserved by the cold temperatures and ends up trapped near the surface (under the sea ice) and gets sometimes emitted under the form of bubbles. Such emissions are still poorly characterized.

Understanding better the sources in the Artic is crucial as any additional emissions from Arctic regions may intensify global warming through climatic positive feedback. In this study we want to characterize the methane transport from different sources, as observed from the Academician Mstislav Keldysh“ (AMK) ship during its cruise of Septembers 2022 in the Murmansk-Kara Sea. To track the atmospheric transport, we use FLEXPART backward trajectories along the ship cruise, using ERA5 global data at 0.5 degrees resolution as meteorological input data. We release 10,000 backtrajectories from a 3D box of 0.1° x 0.1° x 90m in a point centered around the ship position, chosen every 6 hours along the ship track for the whole campaign. The trajectories travel back in time for 2 months, to consider also for long range sources. In addition, we take into consideration the background concentrations from air masses older than 2 months, by using the 3D concentrations simulated by FLEXPART-CTM (Chemistry transport model), a model that also take into account some of the basic linear chemical reactions. The results for the campaign of September 2022 are shown in Figure 2:

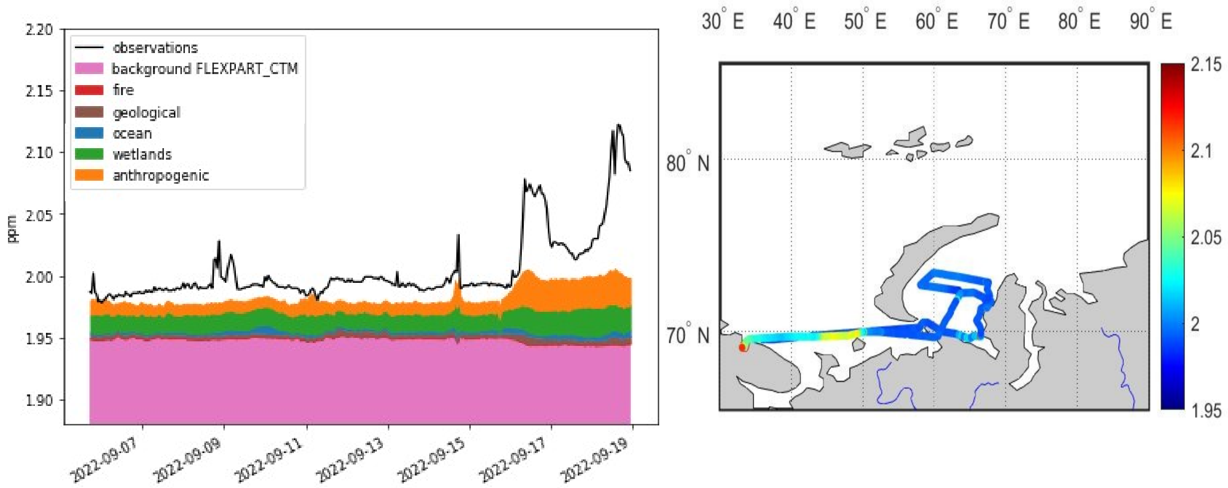

Figure 2: CH_4 concentration as observed by the AMK 89 cruise (in black) compared with the contributions from different emissions: fire (using the Global Fire Emission Database GFED emissions from the Copernicus Atmosphere Monitoring Service CAMS), geological (using emissions from Etiope et al 2019), ocean (emissions from Weber et al 2019), wetlands (emission from WetCHARTs v.1.3.1, Bloom et al 2021) and anthropogenic emissions from CAMS. In the right panel the position of the ship during the cruise, with the corresponding CH4 concentration values.

The analysis confirms how the wetlands constitute in fact the largest contribution to the methane concentrations along the flight (green layer). The background values (in pink) seems to be reasonably reproduced, as when there are peaks dominated by anthropogenic sources (as around the 11 and the 15 September) the modelled values are very close to the observed ones. Several peaks instead seem to be missing in the modelled representation, as around the 9 September and between the 17 and the 19 of September. These peaks can be possibly related to the presence of bubbles as the air in these traits appeared to be transported from the surface of the ocean. Further analysis is planned to include also the results from the oceanographer groups collecting data from the same ship, to see if they observe, in their soundings, possible vertical structure of bubbles. In such case, our analysis will allow to quantify the amount of CH_4 emitted from such events.

4) Transport of microplastics in the atmosphere

Microplastics are an emerging pollutant with environmental as well as human health impacts. These particles have been detected in freshwater and marine environments, in sediment and in sewage sludge. However, research on microplastics in the atmosphere has not kept pace with the study of microplastic pollution in other environmental compartments.

Depending on their size and shape, microplastic particles can be transported long distances in the atmosphere, both vertically and horizontally. Recent modelling studies indicate their presence even in the stratosphere (Tatsii et al., 2024). However, data on the distribution and concentration of microplastics in the stratosphere are currently lacking (Allen et al., 2022).

A quite unknown atmospheric microplastic source is the microplastic resuspension from bare soil regions during mineral dust events. Therefore, we created a global microplastic emission inventory based on the available knowledge regarding the microplastic content in these soils, their respective enrichment in the atmosphere, and the mineral dust fluxes. The total resuspensions were estimated at 104 (48 −110) tonnes yr^{-1}. Based on the calculated resuspensions, we simulated the global atmospheric transport for fiber-shaped plastic particles using FLEXPART. The model was driven by the hourly meteorological re-analysis dataset ERA5 from ECMWF with $0.5^\circ \times 0.5^\circ$ resolution for the year 2018. Output with $1^\circ \times 1^\circ$ resolution was produced every 6 hours. FLEXPART simulations showed that annually, 75 (43−83) tonnes of microfibers are deposited on land and 29 (18−33) tonnes in the oceans. Resuspended microplastics can reach remote regions, such as the Arctic and even some parts of Antarctica.

Furthermore, we estimate the concentration of microplastics from the second largest primary source, road traffic emissions, in the stratosphere and upper troposphere. Road traffic-related emissions of microplastics include those from tires, road markings and polymer-modified bitumen and, according to our estimates, is 4224 kt/year.

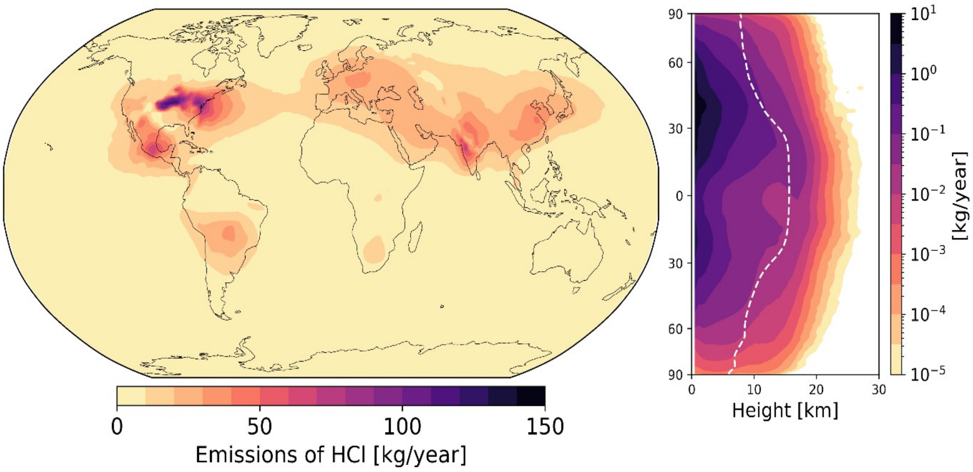

Figure 3: Global emissions of HCl potentially released from halogenated microplastics exposed to UV light in 2014. Left panel: total atmospheric column emissions of HCl; right panel: vertical profile of zonal means of emitted HCl. The white dashed line is the annual mean thermal tropopause.

Microplastic particles degrade and can release halogenated gases such as chlorine when exposed to ultraviolet (UV) light. For example, neoprene, also known as polychloroprene, which is found in tires, contains around 40% chlorine by weight. The released chlorine compounds could be involved in the catalytic destruction of stratospheric ozone, as is the case with the release of chlorofluorocarbons (CFCs) and halons under the Montreal Protocol.

Therefore, we used the Lagrangian particle dispersion model FLEXPART to simulate the atmospheric transport of cylindrical particles of different sizes to understand how much microplastics from the second largest primary source can be found in the upper troposphere and stratosphere, and how much chlorine can potentially be released during UV degradation of microplastics. The simulations used hourly ERA5 reanalysis of global meteorological data. Figure 3 shows the preliminary results for global emissions of HCl as a release from halogenated microplastics related to road traffic emissions.

5) A global re-analysis of regionally resolved emissions and atmospheric mole fractions of SF6 for the period 2005-2021

We employ a global inversion setup to globally determine the distribution of regionally resolved SF_6 emissions between 2005 and 2021 (Vojta, et al. 2024), based on the methodological findings of Vojta et al. 2022. We show a substantial decline in U.S. SF_6 emissions (see Figure 4), indicating the positive effects of national regulation measures. We also find a decreasing emission trend in the EU, with a substantial drop after 2017, likely a result of the EU's 2014 F-gas regulation. Chinese emissions, however, show a strong positive trend that is even higher than the average global total emission trend. We further demonstrate that national reports to the United Nations Framework Convention on Climate Change underestimated the SF_6 emissions in the U.S., EU, and China throughout the whole study period. The aggregation of all the regionally resolved emissions shows a relatively good agreement with total global emissions, however, results are sensitive to the employed a priori emission fields, likely due to the challenges in constraining emissions in regions poorly covered by the observation network. Lastly, monthly inversion results show higher SF_6 emissions in summer than in winter in the Northern Hemisphere.

In this project, we used the hourly meteorological re-analysis dataset ERA5 from ECMWF for two purposes: (1) the Lagrangian particle dispersion model FLEXPART was driven with ERA5 to calculate the source-receptor relationship on which the inversion is based on, and (2) ERA5 was used to perform a global re-analysis of SF_6 for the years between 2005 and 2021 in order to estimate the background.

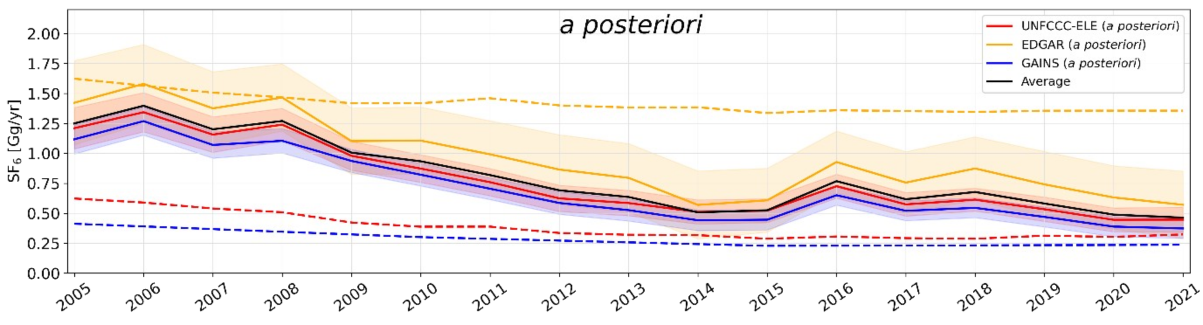

Figure 4: . Annual a priori (dashed lines) and a posteriori (solid lines) SF_6 emissions in the U.S. for the period between 2005 and 2021 when using different a priori inventories (UNFCCC-ELE red, EDGAR orange, GAINS blue). The a posteriori emissions are shown together with their respective 2-σ uncertainties (colored shadings) and the black solid line represents the average of the three different a posteriori emissions.

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