

CLIMATE CHANGE

12/2026

Final report

Climate Neutrality by 2050

Part 2: Atmospheric data on SF6 and NF3 in Europe and
Germany

by:

Prof. Dr. Andreas Engel, Katharina Meixner

Goethe Universität Frankfurt Am Main. Institut für Atmosphäre und Umwelt, Frankfurt/M.

publisher:

German Environment Agency

CLIMATE CHANGE 12/2026

AA-Forschungsplan of the Federal Foreign Office

Project No. (FKZ) 3722 41 301 2

FB001943/ENG

Final report

Climate Neutrality by 2050

Part 2: Atmospheric data on SF₆ and NF₃ in Europe and Germany

by

Prof. Dr. Andreas Engel, Katharina Meixner

Goethe Universität Frankfurt Am Main. Institut für
Atmosphäre und Umwelt, Frankfurt/M.

On behalf of the German Environment Agency

Imprint

Publisher

Umweltbundesamt
Wörlitzer Platz 1
06844 Dessau-Roßlau
Tel: +49 340-2103-0
Fax: +49 340-2103-2285
buergerservice@uba.de
Internet: www.umweltbundesamt.de

Report performed by:

Institute for Atmospheric and Environmental Sciences, Goethe University Frankfurt
Altenhoferallee 1
60438 Frankfurt am Main
Germany

Report completed in:

October 2025

Edited by:

Section III 1.4 Substances-related Product Issues
Dr. Cornelia Elsner

DOI:

<https://doi.org/10.60810/openumwelt-8173>

ISSN 1862-4359

Dessau-Roßlau, April 2026

The responsibility for the content of this publication lies with the author(s).

Abstract: Climate Neutrality by 2050: part 2 Atmospheric data on SF₆ and NF₃ in Europe and Germany

The project focused on the investigation of the greenhouse gases SF₆ (sulfur hexafluoride) and NF₃ (nitrogen trifluoride) was divided into three work packages. The aim of the first work package was to compile all available measurements of SF₆ in Germany into a consistent dataset. This included ensuring uniform calibration scales and data homogeneity. The second work package investigated these datasets for pollution events that could indicate regional emissions. The third work package concentrated on initiating the first measurements of NF₃ in Germany, as there were no routine measurements of this gas prior to the project.

SF₆ and NF₃ are long-lived greenhouse gases with extremely high global warming potentials (GWP-100 values of 23,500 and 16,100). Their use, especially in switchgear and in the semiconductor industry, has led to a significant rise in their atmospheric mixing ratios globally. Before the project commenced, SF₆ was regularly measured at only two stations of the Federal Environment Agency (UBA), while NF₃ was deemed very challenging to measure. Progress in SF₆ measurement technique was made, revealing that the highest European emission occur in Germany, in particular in a region in Baden-Württemberg.

As part of the project, regular measurements of both SF₆ and NF₃ were established at the Taunus Observatory of Goethe University Frankfurt, utilizing modern technologies to enhance measurement accuracy and precision. The measurements at Taunus Observatory are fully incorporated into the AGAGE network. A comprehensive data integration process, using various measurement stations across Germany, allowed for a detailed analysis of emissions.

Initial results from NF₃ measurements indicated that background concentrations increased from 3.3 ppt in February 2023 to 4.0 ppt by February 2025, with very few significant pollution events occurring. The findings suggested that the local sources of NF₃ emissions are quite small, and quantifying emissions was deemed unreliable due to the limited number of events.

In summary, the project aims to enhance the understanding of SF₆ and NF₃ emissions in Germany by creating a consistent, high-quality dataset that contributes to identifying and analyzing emission sources.

Kurzbeschreibung: Klimaneutralität bis 2025: Teilvorhaben 2 Auswertung von Atmosphärendaten von SF₆ und NF₃ im Europäischen Raum

Das Projekt zur Untersuchung der Treibhausgase SF₆ (Schwefelhexafluorid) und NF₃ (Nitrogen trifluorid) wurde in drei Arbeitspakete unterteilt. Ziel des ersten Arbeitspakets war die Zusammenstellung aller verfügbaren Messdaten von SF₆ in Deutschland, um eine konsistente Datenbasis zu schaffen. Dies umfasste die Sicherstellung einheitlicher Kalibrierungsmaßstäbe und die Homogenität der Daten. Im zweiten Arbeitspaket wurden diese Daten untersucht, um Verschmutzungsepisoden zu identifizieren, die auf regionale Emissionen hindeuten könnten. Das dritte Arbeitspaket konzentrierte sich auf die Ersterfassung von NF₃ in Deutschland, da zuvor keine regelmäßigen Messungen dieses Gases existierten.

SF₆ und NF₃ sind langlebige Treibhausgase mit extrem hohen globalen Erwärmungspotenzialen (GWP-100-Werte von 23.500 und 16.100). Die Verwendung dieser Gase, insbesondere in Schaltanlagen und in der Halbleiterindustrie, führte zu einem signifikanten Anstieg der Mischungsverhältnisse in der globalen Atmosphäre. Vor Beginn des Projekts wurden SF₆-Messungen nur an zwei Stationen des Umweltbundesamtes (UBA) durchgeführt, während NF₃ als äußerst schwer messbar galt. Fortschritte in der Messung von SF₆ wurden erzielt, und es

wurde festgestellt, dass die höchsten europäischen Emissionen in Deutschland abgeleitet wurden, insbesondere über einer Region in Baden-Württemberg.

Im Rahmen des Projekts wurden regelmäßige Messungen sowohl von SF₆ als auch NF₃ am Taunusobservatorium der Goethe-Universität Frankfurt etabliert, wobei moderne Technologien eingesetzt wurden, um die Genauigkeit und Präzision der Messungen zu verbessern. Die Messungen sind vollständig in das internationale AGAGE Netzwerk eingebunden. Eine umfassende Datenintegration mithilfe von verschiedenen Messstationen in Deutschland ermöglichte eine differenzierte Analyse der Emissionen.

Die ersten Ergebnisse der NF₃-Messungen zeigen, dass die Hintergrundkonzentrationen von NF₃ von 3,3 ppt im Februar 2023 auf 4,0 ppt bis Februar 2025 angestiegen sind, wobei nur wenige signifikante Verschmutzungsereignisse auftraten. Die Resultate deuteten darauf hin, dass die Quellen der NF₃-Emissionen regional gering sind und eine Quantifizierung der Emissionen aufgrund der geringen Anzahl an Ereignissen als unzuverlässig angesehen wurde.

Zusammenfassend zielt das Projekt darauf ab, das Verständnis der Emissionen von SF₆ und NF₃ in Deutschland zu verbessern, indem eine konsistente, qualitativ hochwertige Datenbasis geschaffen wird, die zur Identifizierung und Analyse von Emissionsquellen beiträgt.

Table of content

List of figures	8
List of tables	8
List of abbreviations	9
Summary	10
Zusammenfassung.....	10
1 General Motivation and Outline.....	16
2 An improved data base on SF ₆ in ambient air over Germany	18
3 Pollution Events and German emission estimate of SF ₆	24
3.1 General approach.....	24
3.2 Inverse modelling study of German and European SF ₆ emissions using InTEM.....	24
3.3 Uncertainty of emission estimates.....	30
4 First observations of NF ₃ over Germany.....	34
5 List of references	36

List of figures

Figure 1:	SF ₆ measurements at German ICOS stations.....	20
Figure 2:	SF ₆ measurements at Zugspitze and Taunus Observatory	21
Figure 3:	Monthly average SF ₆ background mole fractions at German station used in this report	22
Figure 4:	Distribution of European stations used in this study	22
Figure 5:	Distribution of German SF ₆ Emissions derived from InTEM for the years 2020-2023.....	26
Figure 6:	Comparison of observations and model	27
Figure 7:	German SF ₆ emission estimates (top-down)	28
Figure 8:	Reported German SF ₆ emissions	29
Figure 9:	Prior distribution distribution of German annual average SF ₆ Emissions based on EDGAR emissions distributed according to population density	32
Figure 10:	Distribution of German SF ₆ Emissions derived from InTEM for the years 2020-2023 with reduced data base.....	33
Figure 11:	First Chromatogram of NF ₃ from the new Medusa system at Taunus Observatory.	34
Figure 12:	time series of NF ₃ from the new Medusa system at Taunus Observatory.....	35

List of tables

Table 1:	Comparison of top-down (InTEM and Flexinvert) derived emissions of SF ₆ with bottom up emission from EDGAR and emissions reported to UNFCC.	30
----------	---	----

List of abbreviations

Abbreviation	Explanation
SF ₆	Sulfur hexafluoride
NF ₃	Nitrogen trifluoride
UNFCCC	United Nations Framework Convention on Climate Change
SIO	SCRIPPS Institute of Oceanography
AGAGE	Advanced Global Atmospheric Gas Experiment
ECD	Electron Capture Detector
NOAA	National Oceanographic and Atmospheric Administration
ICOS	Integrated Carbon Observing System
UBA	Umweltbundesamt
NAME	Numerical Atmospheric dispersion Modelling Environment
EDGAR	Emissions Database for Global Atmospheric Research
ppt	Parts per trillion
InTEM	Inversion Technique for Emission Modelling
NAME	Numerical Atmospheric Dispersion Modelling Environment

Summary

The present report documents a project that addresses the distribution of SF₆ and NF₃ in Germany and the emissions of SF₆. Two of the three work packages focus on the greenhouse gas SF₆ (sulfur hexafluoride), while one focuses on NF₃ (nitrogen trifluoride). The primary goal of the first work package was to gather all available measurement data on SF₆ in Germany and compile them into a consistent dataset. This involved ensuring consistent calibration scales as well as ensuring the homogeneity of the data. In the second work package, an analysis of the collected data was conducted to identify pollution events that could indicate regional emissions. The third work package focused on the first measurements of NF₃ in Germany, as no measurements of this greenhouse gas had been conducted in Germany previously.

SF₆ and NF₃ are two fully fluorinated greenhouse gases with extremely high global warming potentials (GWP-100) of 23,500 and 16,100, respectively. Both gases are used in the semiconductor industry, with SF₆ primarily utilized in switchgear and, specifically in Germany, was incorporated into soundproof windows. Before the project commenced, SF₆ was only regularly measured at two monitoring stations of the Federal Environment Agency (UBA) in Germany: at Zugspitze and on Schauinsland near Freiburg. Additionally, SF₆ is regularly measured as part of the ICOS program from samples collected at various stations. Measuring NF₃ poses a particular experimental challenge due to its very low boiling point, low concentration in the atmosphere, and cross-interferences with other substances, resulting in no previous measurements of NF₃. In February 2023, a so-called MEDUSA measurement system was installed at the Taunus Observatory, which can accurately measure SF₆ and NF₃ alongside a large range of halogenated hydrocarbons. The measurements at the Taunus Observatory are part of the AGAGE network, which conducts regular data reviews for quality assurance.

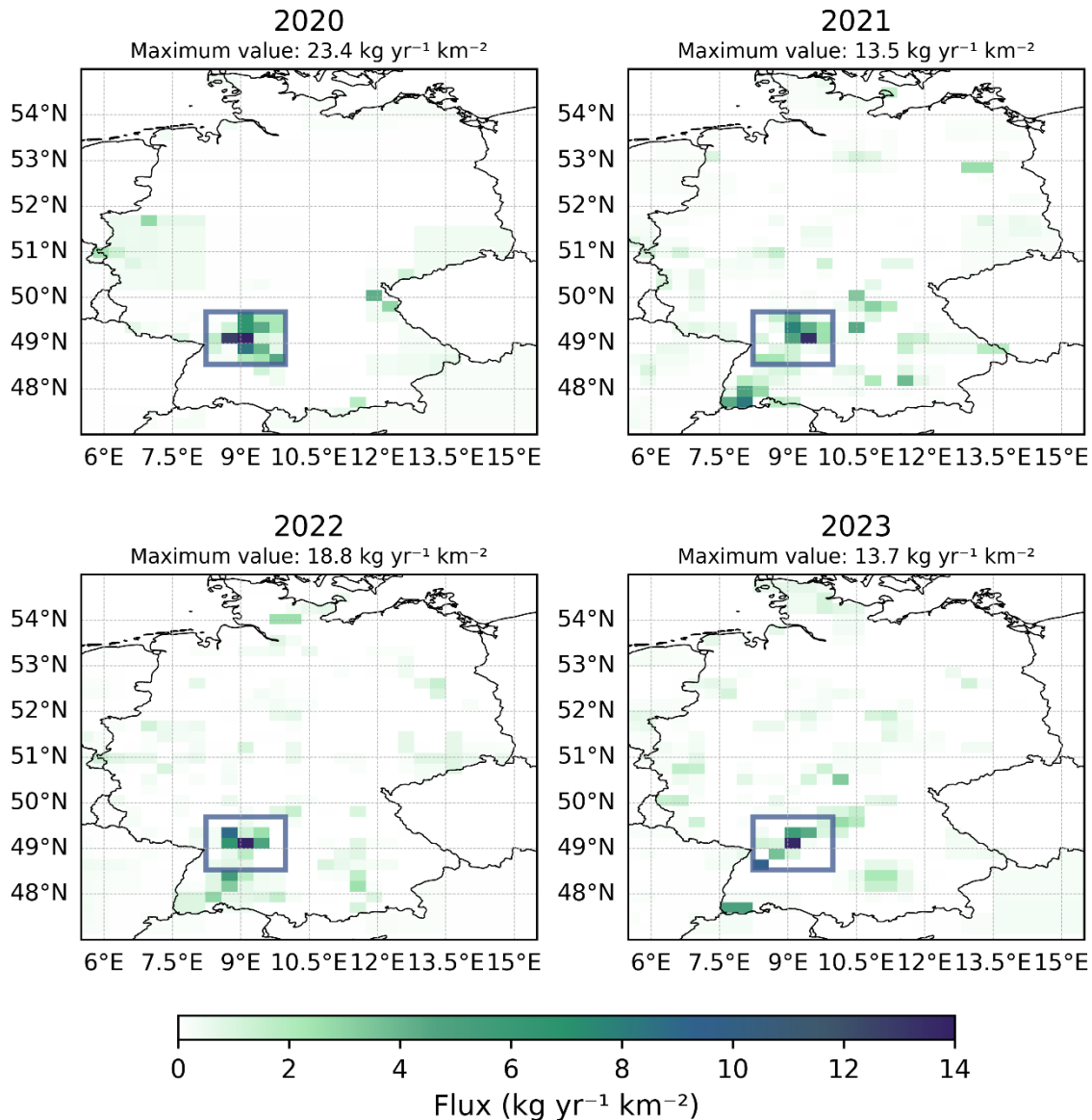
As part of the project, extensive data on SF₆ in Germany were compiled from various sources. Key sources included the Zugspitze measurement station of the UBA as well as the Taunus Observatory of Goethe University in Frankfurt. Moreover, additional measurement series from ICOS (Integrated Carbon Observation System) in Germany were integrated; however, these have a significantly lower temporal resolution. All measurements were conducted using gas chromatography, employing both mass spectrometric (MS) and electron capture detection (ECD) methods. To ensure comparability of the data, all data were converted to a consistent calibration scale. It was found that particularly high episodic mixing ratios of SF₆ were observed at two German stations (Taunus Observatory and Karlsruhe), which suggest a regional source in southwestern Germany. The monthly averaged background values calculated in the project show good agreement at all stations, indicating high data quality.

During the project, the opportunity arose to collaborate with the UK Met Office to perform what is known as an inverse calculation. In this process, the InTEM model is used, which combines an inversion with the numerical atmospheric transport model NAME (Numerical Atmospheric Dispersion Modelling Environment). A predefined emission field (so-called a priori assumption) is coupled with the atmospheric transport model to generate time series of the expected mixing ratios at the available measurement stations. This emission field is then optimized within a mathematical procedure to achieve the best possible agreement between the model and observations. The resulting emission field (a posteriori) shows the emissions that best explain the observations.

The resulting emission fields for the years 2020-2023 all exhibit a very inhomogeneous distribution of emissions, with a hotspot identified in the southwestern region of Germany. Emissions from this region for 2020 were estimated to be 59±16 tons per year, and for the years 2021-2023, they were estimated to be between 29±11 and 35±13 tons per year.

SF₆ Emissions derived from atmospheric observations

Annual mean emissions for Germany for the years 2020 to 2023 derived by the InTEM model based on atmospheric observations.



Annual mean inversely derived emissions of SF₆ for Germany from 2020 to 2023. The defined focus area shows a region with particularly high emissions in southwestern Germany. [source: Meixner et al., 2025]

This region with particularly high emissions cannot be reconciled with the presumed German emission sources for SF₆. It is assumed that the main source is SF₆-insulated soundproof windows, from which the enclosed SF₆ escapes during disassembly/scraping. Such a source should, however, be largely homogeneously distributed across Germany or scale with population density. Despite this discrepancy, the total emissions derived from the modeling calculations for Germany are in good agreement with the total emissions reported to the UNFCCC. This suggests that the reported values may not adequately reflect the distribution of actual emissions, particularly if emissions from point sources are not considered in the official reports.

Another aim was to measure NF₃. NF₃ poses a particular challenge for measurement due to its physicochemical properties. With a very low boiling point of -129 °C, low atmospheric concentration, and cross-interferences with other gases, measuring it is complicated. In February 2023, the MEDUSA system was installed at the Taunus Observatory, which allows for the measurement of NF₃. Initial measurements showed a concentration of 3.3 ppt in early 2023, which had increased to approximately 4.2 ppt by mid-2025. The increase is not necessarily related to local or regional factors, as NF₃ has a long atmospheric lifetime of over 500 years. Since there are few observed spikes in the measured mixing ratios above the background value, it can be inferred that sources of NF₃ in the region are low. Only three significant spikes were observed in the measurement series.

Overall, the results highlight that the continuous measurements of NF₃ and SF₆ at the Taunus Observatory provide valuable data for monitoring emissions in Germany. This information is crucial for future research efforts and for improving emission inventories. In summary, the report illustrates the progress made in data collection and analysis of SF₆ and NF₃ emissions in Germany. The results underscore the necessity of creating comprehensive and consistent datasets to enable a better understanding of emissions and their sources. The project has laid the groundwork for future studies to further investigate the regional distribution and temporal development of both mixing ratios and emissions of these greenhouse gases in Germany. This is deemed an important step in better understanding of sources of greenhouse gas emissions, which is a prerequisite in their effective reduction.

Zusammenfassung

Der vorliegende Bericht dokumentiert ein Projekt, welches sich mit der Verteilung von SF₆ und NF₃ in Deutschland und den Emissionen von SF₆ beschäftigt. Zwei der drei Arbeitspakete konzentrieren sich auf das Treibhausgas SF₆ (Schwefelhexafluorid), während sich eines auf NF₃ (Stickstofftrifluorid) konzentriert. Das Hauptziel des ersten Arbeitspakets bestand darin, alle in Deutschland verfügbaren Messdaten zu SF₆ zu sammeln und in einem konsistenten Datensatz zusammenzuführen. Dies umfasste die Sicherstellung konsistenter Kalibrationsskalen sowie die Gewährleistung der Homogenität der Daten. Im zweiten Arbeitspaket wurde eine Analyse der gesammelten Daten durchgeführt, um Verschmutzungsereignisse zu identifizieren, die auf regionale Emissionen hindeuten könnten. Das dritte Arbeitspaket konzentrierte sich auf die ersten Messungen von NF₃ in Deutschland, da zuvor keine Messungen dieses Treibhausgases in Deutschland stattfanden.

SF₆ und NF₃ sind zwei vollständig fluorierte Treibhausgase mit extrem hohen Treibhauspotenzialen (GWP-100) von 23.500 und 16.100. Beide Gase werden in der Halbleiterindustrie eingesetzt, wobei SF₆ in erster Linie in Schaltanlagen verwendet wird und, speziell in Deutschland, in Schallschutzfenstern verbaut wurde. Vor Beginn des Projekts wurde in Deutschland nur SF₆ an zwei Monitoring-Stationen des Umweltbundesamtes (UBA) regelmäßig gemessen: an der Zugspitze und auf dem Schauinsland, nahe Freiburg. Zusätzlich wird SF₆ regelmäßig im Rahmen des ICOS Programms an Proben gemessen die an verschiedenen Stationen gesammelt werden. Die Messung von NF₃ erweist sich als besondere experimentelle Herausforderung aufgrund seines sehr niedrigen Siedepunkts, seiner geringen Konzentration in der Atmosphäre und Querinterferenzen mit anderen Substanzen, so dass es keine Messungen von NF₃ gab. Im Februar 2023 wurde ein sogenanntes Medusa Messsystem am Taunus Observatorium installiert, welches neben einer Vielzahl halogenierter Kohlenwasserstoffe auch SF₆ und NF₃ mit hervorragender Präzision messen kann. Die Messungen am Taunus-Observatorium sind Teil des AGAGE-Netzwerks, welches regelmäßige Datenüberprüfungen zur Qualitätssicherung durchführt.

Im Rahmen des Projekts wurden umfassende Daten aus verschiedenen Quellen über SF₆ in Deutschland zusammengetragen. Zu den wichtigsten Quellen zählen die Messstation Zugspitze des UBA sowie das Taunus-Observatorium der Goethe-Universität Frankfurt. Zusätzlich wurden neue Messreihen von ICOS (Integrated Carbon Observation System) in Deutschland integriert, die jedoch eine wesentlich niedrigere zeitliche Auflösung aufweisen. Alle Messungen wurden mithilfe der Gaschromatographie durchgeführt, wobei sowohl massenspektrometrische (MS) als auch Elektroneneinfangdetektoren (ECD) eingesetzt wurden. Um die Vergleichbarkeit der Daten zu gewährleisten, wurde alle Daten auf eine konsistente Kalibrationsskala umgerechnet. Es zeigte sich, dass insbesondere an zwei deutschen Stationen (Taunus Observatorium und Karlsruhe) episodisch besonders hohe Mischungsverhältnisse von SF₆ beobachtet wurden, die auf eine regionale Quelle im Süd-Westen Deutschlands hindeuten. Die monatlich gemittelten Hintergrundwerte an allen Stationen die im Projekt berechnet wurden stimmen hingegen gut überein, was die hohe Datenqualität zeigt.

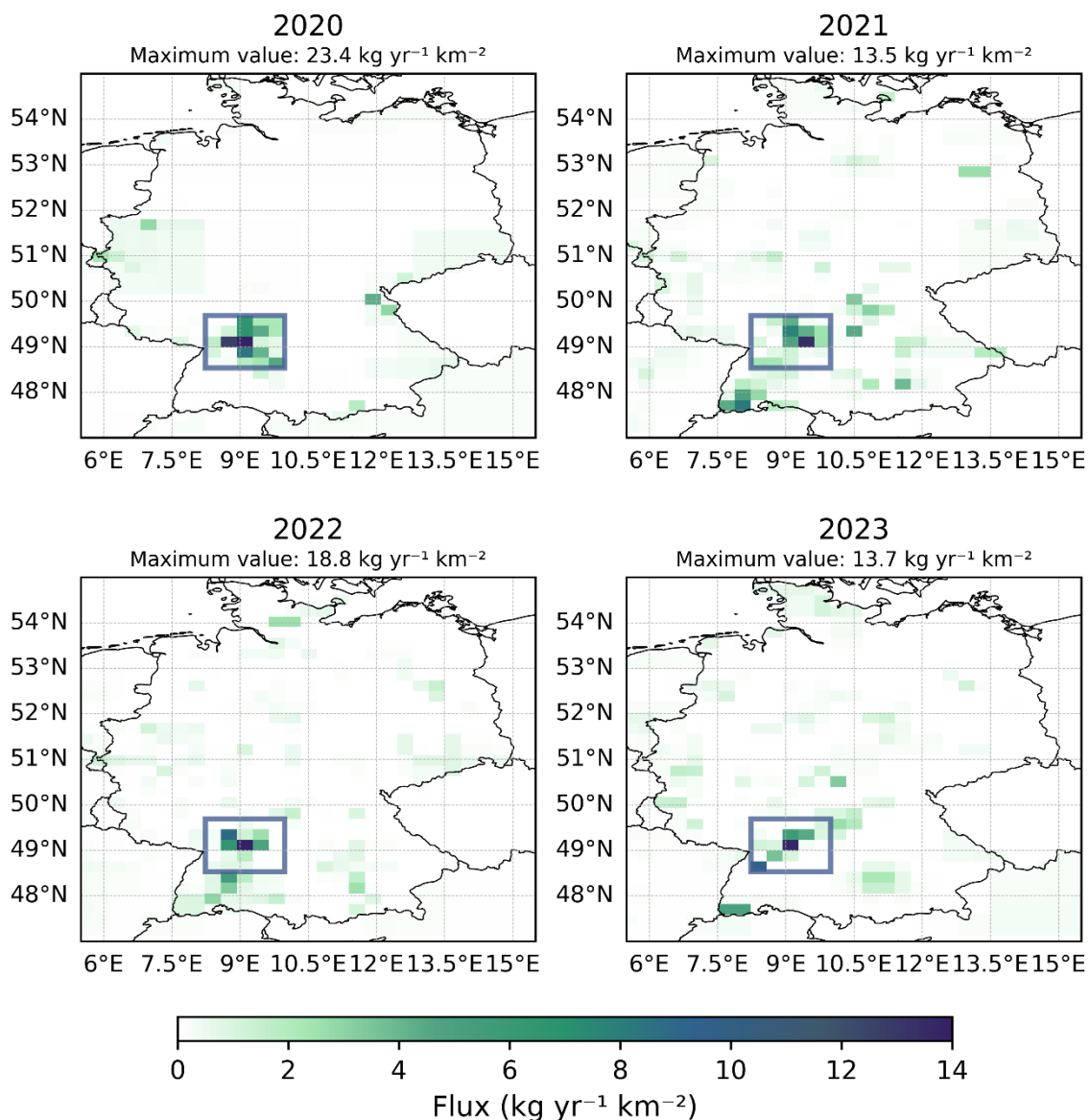
Im Laufe des Projektes ergab sich die Möglichkeit in Zusammenarbeit mit dem UK Met Office eine sogenannte inverse durchzuführen. Hierbei wird das InTEM-Modell eingesetzt, welches eine Inversion mit dem numerischen atmosphärischen Transportmodell NAME (Numerical Atmospheric dispersion Modelling Environment) kombiniert. Hierbei wird ein vorgegebenes Emissionsfeld (sogenannte a priori Annahme) mit dem atmosphärischen Transportmodell gekoppelt, um Zeitreihen der erwarteten Mischungsverhältnisse an den vorhandenen Messstationen zu generieren. Dieses Emissionsfeld wird dann im Rahmen eines mathematischen

Verfahrens so optimiert, dass eine bestmögliche Übereinstimmung zwischen Modell und Beobachtungen gefunden wird. Das hieraus resultierende Emissionsfeld (a posteriori) zeigt dann die Emission die die Beobachtungen am besten erklären.

Die sich hieraus ergebenden Emissionsfelder für die Jahre 2020-2023 zeigen alle eine sehr inhomogene Verteilung der Emissionen auf, wobei ein Hotspot in der südwestlichen Region Deutschlands identifiziert wurde. Die Emissionen aus dieser Region für 2020 wurden auf 59 ± 16 Tonnen pro Jahr und für die Jahre 2021-2023 auf 29 ± 11 bis 35 ± 13 Tonnen pro Jahr geschätzt.

Aus Beobachtungen abgeleitete Verteilung der SF₆ Emissionem

Aus atmosphärischen Messungen und dem InTEM Model abgeleitete jährlich gemittelte Emissionen von SF₆ für Deutschland für die Jahre 2020 bis 2023.



Jährliche, mittlere, invers abgeleitete Emissionen von SF₆ für Deutschland von 2020 bis 2023. Das definierte Fokusgebiet zeigt eine Region mit besonders hohen Emissionen in Südwestdeutschland. [source: Meixner et al., 2025]

Diese Region mit besonders hohen Emissionen lässt sich nicht mit den deutschen Emissionsquellen für SF₆ vereinbaren, wie sie an das UNFCCC berichtet werden. Hier wird angenommen, dass die Hauptquelle SF₆-isolierte Schallschutzfenster sind, bei deren Ausbau/Verschrottung das eingeschlossene SF₆ entweicht. Eine solche Quelle sollte allerdings weitgehend homogen in Deutschland verteilt sind, bzw., mit der Bevölkerungsdichte skalieren. Trotz dieser Diskrepanz sind die Gesamtemissionen die für Deutschland aus den Modellrechnungen abgeleitet werden in guter Übereinstimmung mit den Gesamtemissionen die an das UNFCCC berichtet werden. Dies deutet darauf hin, dass die berichteten Werte möglicherweise die tatsächlichen Emissionen nicht ausreichend widerspiegeln, insbesondere wenn die Emissionen aus der Punktquelle nicht in den offiziellen Berichten berücksichtigt sind.

Ein weiteres Ziel stellte die Messung von NF₃ dar. NF₃ stellt aufgrund seiner physikalisch-chemischen Eigenschaften eine besondere Herausforderung in der Messung dar. Mit einem sehr niedrigen Siedepunkt von -129 °C, einer niedrigen Konzentration in der Atmosphäre und aufgrund von Querinterferenzen mit anderen Gasen ist die Messung kompliziert. Im Februar 2023 wurde das MEDUSA-System am Taunus-Observatorium installiert welches auch die Messung von NF₃ ermöglicht. Hiermit wurden die ersten atmosphärischen Messungen von nF₃ in Deutschland initialisiert. Erste Messungen zeigten eine Konzentration von 3,3 ppt Anfang 2023, die bis Mitte 2025 auf ca. 4,2 ppt angestiegen war. Der Anstieg ist nicht unbedingt lokal oder regional bedingt, da NF₃ eine lange atmosphärische Lebensdauer von über 500 Jahren hat. Da es wenige beobachtete Anstiege der gemessenen Mischungsverhältnisse über dem Hintergrundwert gibt, kann zurückgeschlossen werden, dass die Quellen für NF₃ in der Region gering sind. Nur drei signifikante Anstiege wurden in der Messreihe beobachtet.

Insgesamt verdeutlichen die Ergebnisse, dass die kontinuierlichen Messungen von NF₃ und SF₆ am Taunus-Observatorium wertvolle Daten zur Überwachung von Emissionen in Deutschland liefert. Diese Informationen sind entscheidend für zukünftige Forschungsarbeiten und zur Verbesserung der Emissionsinventare.

Zusammenfassend zeigt der Bericht die Fortschritte bei der Datenerhebung und Analyse von SF₆- und NF₃-Emissionen in Deutschland. Die Ergebnisse unterstreichen die Notwendigkeit, umfassende und konsistente Datensätze zu erstellen, um ein besseres Verständnis der Emissionen und deren Quellen zu ermöglichen. Das Projekt hat die Basis für zukünftige Studien gelegt, um die Regionalverteilung und die zeitliche Entwicklung der Verteilung und der Emissionen dieser Treibhausgase in Deutschland weiter zu untersuchen. Solche Untersuchungen sind eine Voraussetzung dafür, die Emissionsquellen von Treibhausgasen besser zu verstehen und somit auch diese Emissionen zu reduzieren.

1 General Motivation and Outline

This project was divided into three work packages, two of which were focussed on SF₆ and one on NF₃. The aim of first work package was to gather all German measurements of SF₆ and compile these into a consistent data set. This included e.g. assuring that consistent calibration scales were applied and ensuring homogeneity of the data. The aim of the second workpackage was then to investigate these observation for pollution events which could hint to regional emissions. Finally, the aim of the third work package was to start first measurements of NF₃ in Germany. Following a brief introduction to NF₃ and SF₆ in the atmosphere, the results are reported in the following by work package.

SF₆ and NF₃ are two fully fluorinated and extremely long-lived greenhouse gases, with extremely high global warming potentials (GWP-100 values of 23,500 and 16,100). NF₃ and SF₆ are used in the semiconductor industry, with SF₆ primarily used in switchgear. Mixing ratios of both substances show a significant and continuous increase in the global atmosphere. Prior to the start of this project, there were no regular measurements of NF₃ in Germany. SF₆ was only regularly and semi-continuously measured in-situ at two monitoring stations of the Federal Environment Agency (Zugspitze and Schauinsland). Additionally, some measurements stations collect bottles which are analysed as part of the ICOS programme, but with much lower temporal resolution. Measuring NF₃ presents a significant experimental challenge due to its very low boiling point and simultaneously very low concentration in the atmosphere (Arnold et al., 2013). SF₆ has a very long lifetime in the atmosphere. This estimate has recently been reduced from the previously assumed 3200 years (Ravishankara et al., 1993) to a value between 850 (Ray et al., 2017) and 1278 (Kovács et al., 2017). However, this has no significant impact on the GWP-100 value. Emissions reported to UNFCCC are significantly lower than the emissions needed to explain the atmospheric increase (Levin et al., 2010; Rigby et al., 2010; Simmonds et al., 2020). This gap can only be explained by emissions that are not reported to the UNFCCC. In recent years, significant progress has been made to locate the regions of these emissions. This is based on the technique of inverse modelling (see e.g. (Manning et al., 2021; Manning et al., 2003). In brief, inverse modelling studies use observed time series of trace gases from one or multiple stations which are divided into a background signal (i.e. measurements largely unperturbed by regional emissions) and pollution events (identified by short-term enhancements above this background). The model then tries to find the emission field which is best able to explain the timing and magnitude of the observed enhancements. This technique is referred to as inverse modelling and the emission derived using this technique are called “top-down”, in contrast to “bottom-up” methods, as are used for reporting to UNFCCC. Recent studies have reported declining top-down emissions of SF₆ in both the U.S. (Hu et al., 2023) and in Europe (Vojta et al., 2025). Concerning European SF₆ emissions Vojta et al. (2025) indicated that the highest European emissions are from Germany. However, it has been found from top-down studies that emissions from China dominate the global emissions and have increased over the last decade (Vojta et al., 2024; An et al., 2024), reaching 5.1 (4.8-5.4) Gg yr⁻¹ in 2021. This accounted for more than half of global emissions that year (An et al., 2024). These studies identified electrical equipment as the major emission source.

Concerning NF₃, there are far less regional studies available for NF₃, but it seems that a significant portion of the sources is located in Southeast Asia (Arnold et al., 2018). (Weng et al., 2024), reported that NF₃ emissions from China increased from 0.95 Gg yr⁻¹ in 2017 to 1.41 Gg yr⁻¹ in 2021, which is an increase by nearly 50% over this period. However, due to the difficulty

in measuring NF₃, very few regional measurements exist and thus the data base is much poorer than for SF₆. To allow for better source attribution, more regional observations are needed.

This project therefore aims to enhance the data set regarding the temporal development and, in the case of SF₆, also the spatial distribution of these two trace gases in Germany. For this purpose, regular measurements of NF₃ have been established at the Taunus Observatory of Goethe University Frankfurt (WP3), and SF₆ measurements at the Taunus Observatory were continued and ported to a more modern instrument allowing a better precision and accuracy. The SF₆ measurements have been integrated with continuous UBA's measurements at the Zugspitze and with flask measurements from other sites in Germany (WP1) and beyond Germany to create a consistent dataset. A regional inversion for the determination of German emissions and their spatial attribution has been performed (WP2).

2 An improved data base on SF₆ in ambient air over Germany

For this project we have gathered data from all sources available to us for observations of SF₆ in Germany. Upon application, reference was made to the two measurement series from the Federal Environment Agency (UBA, Umweltbundesamt) at Zugspitze and Schauinsland and the measurements from Goethe University at the Taunus Observatory (Kleiner Feldberg, near Frankfurt). Meanwhile, it has been found that there are further measurement series in Germany, from ICOS (Integrated Carbon Observatory, <https://www.icos-cp.eu/>). These are not high-resolution, temporally detailed in-situ measurements like those from the University of Frankfurt and the Federal Environment Agency, but rather measurements taken from sample containers. These are regularly conducted by the Max Planck Institute for Biogeochemistry in Jena on ICOS sample containers. The resulting measurement series are available online through the ICOS Carbon Portal (<https://www.icos-cp.eu/observations/carbon-portal>, (Engel et al., 2024). Additional SF₆ measurement from the United Kingdom DECC network, from the AGAGE data archive (Prinn et al., 2025) from and from the World Data Centre for Greenhouse Gases at <https://gaw.kishou.go.jp/> have been used. SF₆ data at the sites TOB (ECD) and CBW is available on the ICOS carbon portal (Engel et al., 2024).

An initial overview of these additional data at the ICOS stations Karlsruhe, Hohenpeissenberg, Lindenberg, Ochsenkopf, Steinkimmen, and Gartow is shown in Fig. 1. Fig. 2 displays the data from the UBA station Zugspitze and the Goethe University Frankfurt. The technique used for measurements of SF₆ is that of gas chromatography, either with mass spectrometric (MS) or electron capture detection (ECD). This is a relative measurement method, i.e. a calibration gas with a known concentration is required in order to determine absolute mixing ratios. These calibration gases are usually supplied from a central calibration laboratory, where the absolute calibration scales are maintained, which are derived from gravimetric or volumetric dilution of the pure compounds. Note that not all data used in our study are taken on the same calibration scale. While the data at Taunus Observatory are on the SIO 2005 scale (Prinn et al., 2018; Simmonds et al., 2020), the data from the ICOS and UBA stations are on two different NOAA scales (https://gml.noaa.gov/ccl/sf6_scale.html). The data on the two different NOAA scales have been converted to the SIO 2005 scale using published conversion factors between the NOAA X2006 and X2014 scales (which are also the WMO scales, see (https://gml.noaa.gov/ccl/sf6_scale.html) and from the NOAA scale to the SIO scale (Prinn et al., 2018). The conversion function for the NOAA scales is:

$$SF6_{X2014} = 2.6821 \cdot 10^{-3} \cdot (SF6_{X2006})^2 + 9.7748 \cdot 10^{-1} SF6_{X2006} + 3.5831 \cdot 10^{-2}$$

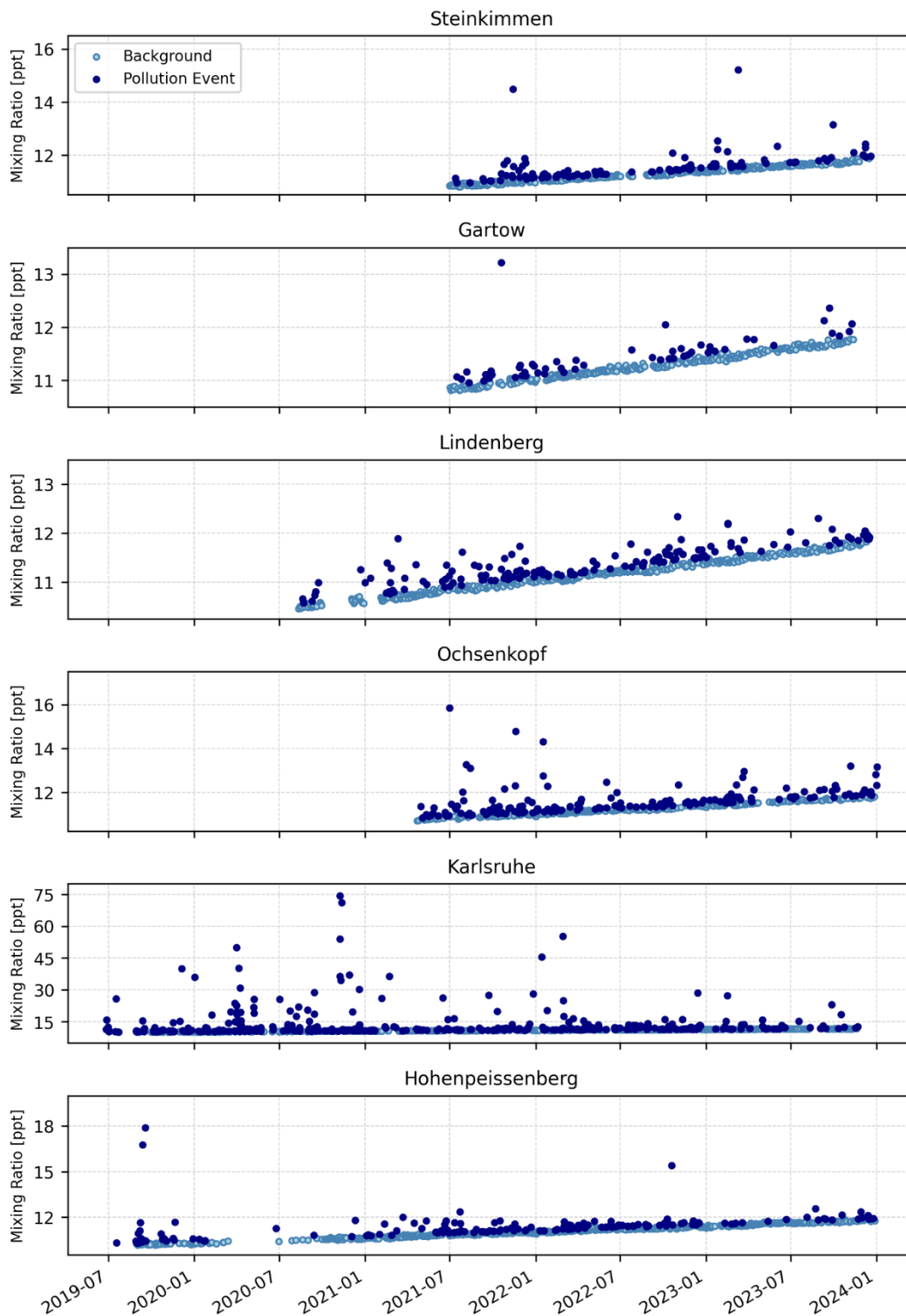
With all SF₆ values in ppt. Note that these conversion are small (usually on the order of 0.5%, but his assures that the data from the different stations are directly comparable. For the Taunus Observatory, the data up to January 2023 was collected using an ECD system, and from January 2023 onwards, additional data from a so called Medusa system (Miller et al., 2008; Arnold et al., 2012) are available . Medusa is a fully automated gas chromatography/mass spectrometric measurement system designed for ultra-high precision measurement of atmospheric trace gases. Since the Medusa data integrates over a period of approximately 20 minutes, whereas the ECD data shows a "snapshot," the pollution episodes in both datasets are not directly comparable , as the shorter sampling interval of the ECD system is expected to show more variability than the Medusa system which averages over 20 minutes. Note that for the inversion presented later in this report we use 4-hour averages of the data, so that such effects are averaged out The data

from the Schauinsland station are not included here, as they contain irregular jumps in the current version that are considered unrealistic. No resources were available to rework these data such that they could be used in this study. Therefore, they are not further investigated here. The other data used in this study have typical precision which are on the order of 0.3% for the Medusa system and below 1% for the ECD measurements. Absolute uncertainties between the different calibration scales are below 0.5%. From Figures 1 and 2, it is clear that the stations Karlsruhe and Taunus show the highest pollution events, which aligns with the assumption of an SF₆ source in southwestern Germany. After the data was divided into background and pollution components, the monthly averages from the background data were calculated and compared. This comparison is shown in Figure 3. There is generally good agreement. Only the SF₆ values from the ECD measurements at the Taunus Observatory exhibit a somewhat higher spread, which is explained by a combination of somewhat poorer precision (up to 1%, 1 sigma standard deviation) and the short sampling interval. Especially the Medusa data taken at Taunus Observatory since February 2023 are subject to continuous data quality control. Regular (every second year) new calibration gas tanks are supplied by the SCRIPPS Institute of Oceanography (SIO) in La Jolla, California, and the data are subject to a half-annual data review within the AGAGE (Advanced Global Atmospheric Gas Experiment, (Prinn et al., 2018)) community. The Taunus Observatory is a full member of the AGAGE global network since February 2023 when the Medusa system was installed.

Next to these data from Germany, data both from ICOS and from AGAGE are available for Europe, which have been incorporated in the inversions and the discussion of emissions presented in WP2. Fig 4. Shows the distribution of all stations available. Different stations have different measurement characteristics. For instance, Zugspitze is a high altitude mountain station which mainly receives clean high-altitude air. It is therefore particularly useful to determine the atmospheric background mixing ratios of long-lived gases like e.g. SF₆. The Taunus Observatory is situated much closer to possible pollution sources and due to its lower altitude will receive more anthropogenically polluted air, as discussed later in this report.

Figure 1: SF₆ measurements at German ICOS stations

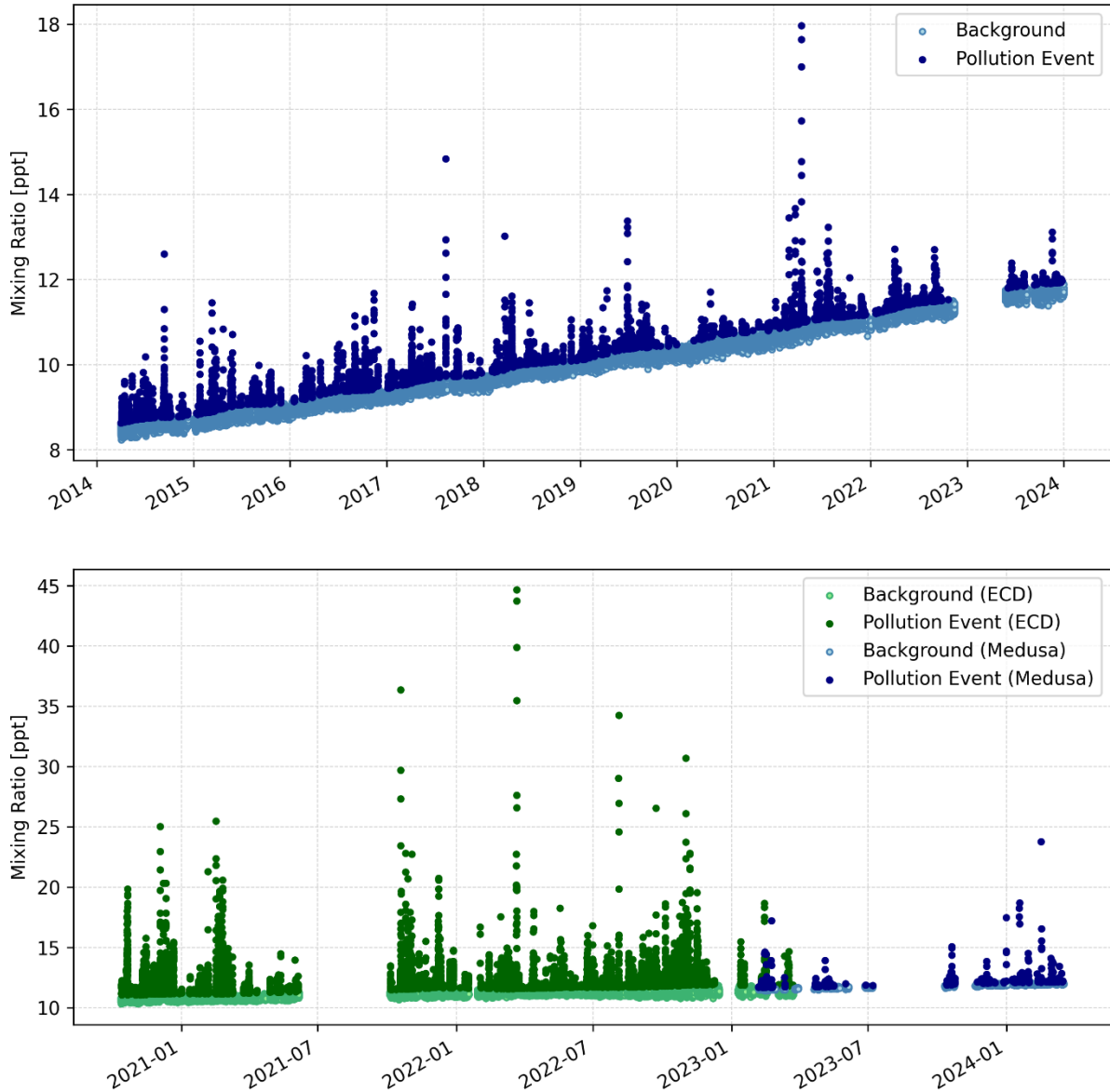
Measurements of SF₆ at various ICOS stations (data from <https://www.icos-cp.eu/observations/carbon-portal>). The division into background and pollution was carried out using a data filter developed at the University of Frankfurt (Schuck et al., 2023).



Source: [Meixner et al., 2025]

Figure 2: SF₆ measurements at Zugspitze and Taunus Observatory

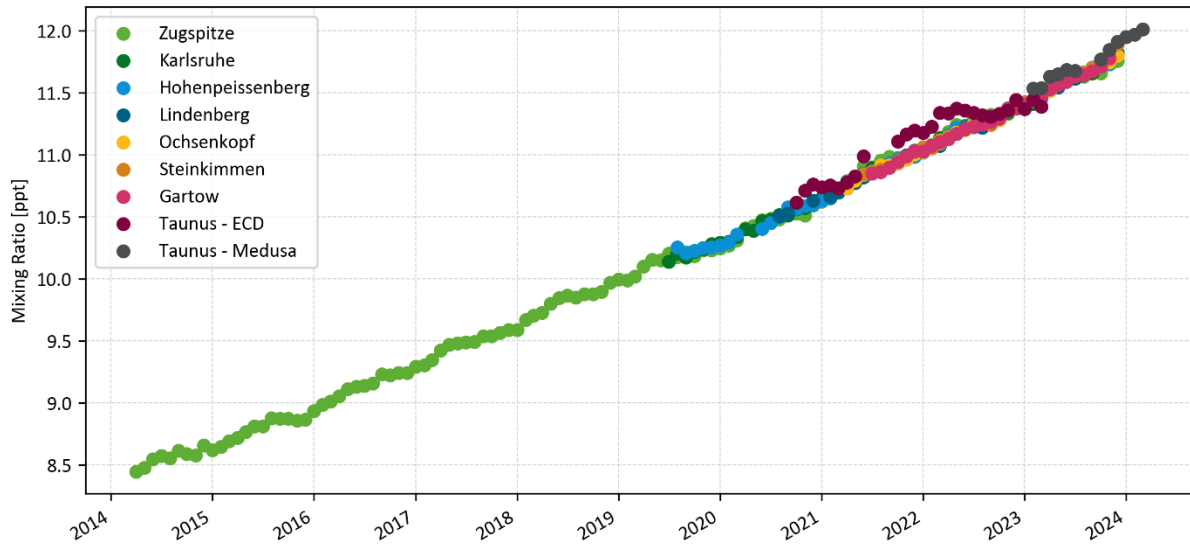
Measurements of SF₆ at the Zugspitze station (top, Federal Environment Agency) and Taunus Observatory (bottom, Goethe University Frankfurt). The division into background and pollution was carried out using a data filter developed at the University of Frankfurt (Schuck et al., 2023). Using the statistical baseline on the Taunus Observatory data, we found that 82% of all measurements were classified as baseline, while 18% were classified as pollution events.



Source: [Meixner et al., 2025]

Figure 3: Monthly average SF₆ background mole fractions at German station used in this report

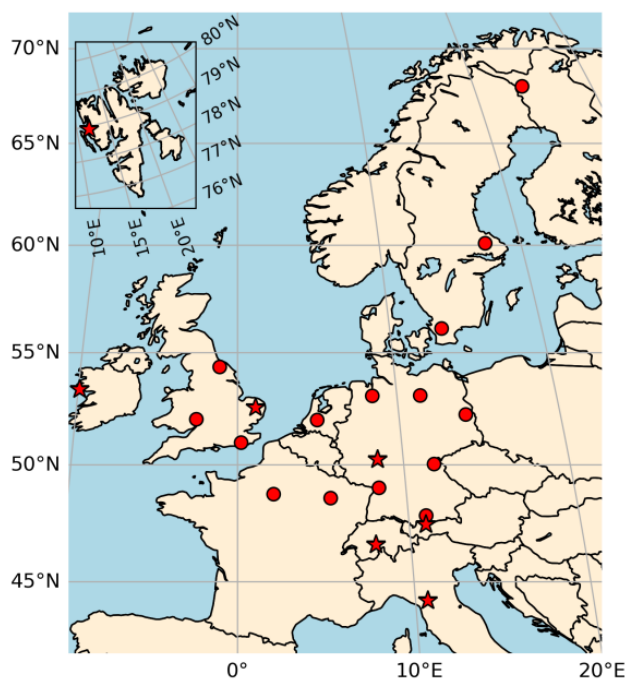
Comparison of background values (monthly averages) from all measurement stations in Germany where SF₆ is regularly measured. The division into background and pollution was carried out using a data filter developed at the University of Frankfurt (Schuck et al., 2023). It should be noted that the raw data from the Taunus Observatory are on a different scale (SIO 05) than the other data (WMO-SF₆-X2014). However, the difference between the scales is less than 1% (1.0049 ± 0.0029) (Prinn et al., 2018). For comparison purposes, all data have been converted to the SIO-05 scale.



Source: [own illustration, Goethe University Frankfurt]

Figure 4: Distribution of European stations used in this study

Spatial distribution of available measurement stations with high-quality SF₆ data. Stars mark continuously measuring stations; circles indicate the stations where air samples are taken that are collected as part of ICOS (data available at <https://www.icos-cp.eu/observations/carbon-portal>), as well as AGAGE or the DECC network in the United Kingdom. The two German stations where high-resolution SF₆ data are collected are the Taunus Observatory (Goethe University Frankfurt) and the measurement station Zugspitze (Federal Environment Agency).



Source: [Meixner et al., 2025]

3 Pollution Events and German emission estimate of SF₆

3.1 General approach

The initial plan for this project was to conduct a statistical evaluation of pollution events of the SF₆ measurements, i.e. separating the data into polluted/unpolluted and looking at statistics of this ratio. However, as the project progressed, the opportunity arose to perform a so-called inversion calculation in addition to such an outlier analysis, leading to an expansion of the work program in this regard. This investigation was triggered by the observation that nowhere in Europe larger pollution of SF₆ was observed than at the German stations, particularly those at the Taunus Observatory and at Karlsruhe. The inversion calculation was carried out in collaboration with A. Manning (UKMet Office) using the InTEM modelling system (Manning et al., 2021). In this method, a so-called a priori assumption about emissions (so-called prior) and a meteorological transport model (NAME) are used to calculate the expected mixing ratios at the available measurement stations. Through optimization, the emission field is adjusted to achieve the best possible agreement between measurement and modelling. The emission field which best matches the observations is then assumed to best represent the real emissions. Note that, in order to get some statistics, the assumption of constant emission over a certain time period needs to be made in these calculations. Previous inversion calculations (Simmonds et al., 2020; Vojta et al., 2024), had already identified the south-western part of Germany as the strongest emissions region in Europe. This was again corroborated in a very recent study (Vojta et al., 2025) using a completely independent inversion scheme (i.e. different inverse models, different meteorological analysis) from the one used in our study. Specifically, we have used the InTEM (Manning et al., 2021) framework described below with meteorological data from the UK Met office unified model, where the study by Vojta used the FlexInvert inversion model with meteorological data from the European Centre for Medium range weather forecast (ECMWF, ERA5 data product). The ERA5 data have a higher temporal and spatial resolution than the UKMet Office data used in our study. A discussion of inverse modelling and the approach of different countries to include inverse modelling, i.e. observation based (so-called top-down) emission estimates in their national reporting can be found in a recent document published by WMO (<https://wmo.int/events/workshop/ig3is-national-scale-applications-of-science-based-quantification-of-emissions-and-removals>).

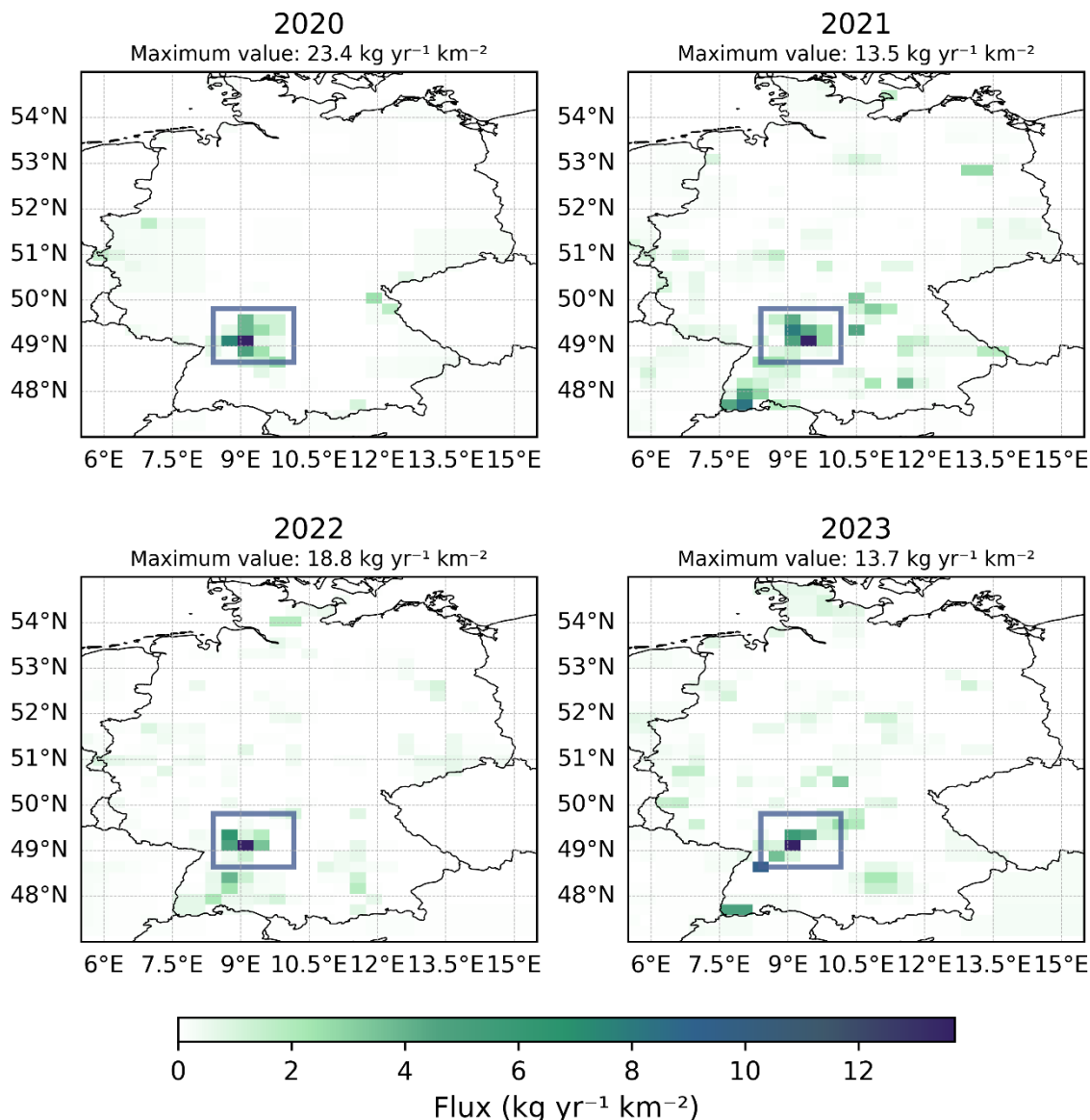
3.2 Inverse modelling study of German and European SF₆ emissions using InTEM

In order to investigate this emission hot spot in more detail, the data set used above was incorporated into the inverse model system InTem in combination with the Lagrangian atmospheric transport model NAME (Numerical Atmospheric dispersion Modelling Environment) as described in Manning et al. (2021) and Meixner et al. (2025). In this setup NAME releases 20,000 particles at each site included in the study per hour. Using the three-dimensional meteorological Unified Model with a resolution of 12 km, these particles are tracked 30 days backwards in time, or until they leave the computational domain, to create source receptor relationships. In NAME, SF₆ is treated as a passive tracer without loss processes. InTEM uses the NAME output from each site to minimise the difference between the computed mole fractions and actual atmospheric observations at the 22 European sites included in our

study. This process is repeated 24 times each time with 10% of the observations removed. Regions in InTEM are initially defined in alignment with national borders and they are further divided within the modelling, based on the impact the different grid cells have at the observation sites. For this study, initial baseline mole fractions were calculated (as described in (Manning et al., 2021) at the AGAGE stations Mace Head (MHD) in Ireland, Jungfraujoch (JFJ) in Switzerland, Monte Cimone (CMN) in Italy and Zeppelin (ZEP) in Norway (Spitsbergen), with the remaining sites using the MHD baseline. Adjustments from the 11 boundary regions surrounding the computational domain then result in unique baselines at each site, with each station having a further freedom within the modelling to allow a small bias from other sites. The EDGAR v8 (Emissions Database for Global Atmospheric Research -- EDGARv8.0) country totals were evenly distributed across each country as the prior emission value. EDGAR uses a technology-based emission factor approach that utilises country-specific activity data, the mix of technology in each sector, abatement measures, emission factors and the reduction by abatement to estimate the emissions of various greenhouse gases and ozone-depleting substances. Global emission estimated by EDGAR were shown to have a satisfactory agreement with globally derived emissions (Levin et al., 2010; Simmonds et al., 2020). Emission estimates from InTEM were derived for three-month periods: January to March, April to June, July to September, and October to December and the results were averaged to determine the annual SF₆ emissions for the years 2020 to 2023. For further details on the method, the resolution and meteorological data used, the reader is referred to Manning et al. (2021) and Meixner et al. (2025). The results of this inversion calculation, taking into account all the measurement stations shown in Fig. 4, are presented in Fig. 5 for the years 2020-2023. It is evident that there is a region with particularly high emissions in the southwestern part of Germany, specifically in the state of Baden-Württemberg. This regional emission hotspot aligns with previous inversion calculations (Simmonds et al., 2020; Vojta et al., 2024, Vojta et al., 2025), also identified this region as an emission hot-spot. To investigate this high-emission region in greater detail, we defined a focus region (48.637°N - 49.807°N, 8.404°E - 10.164°E).

Figure 5: Distribution of German SF₆ Emissions derived from InTEM for the years 2020-2023

Annual mean InTEM derived emissions for Germany for the years 2020 to 2023. The focus area defined in the text is shown as a blue box covering a region with especially high emissions in south-western Germany (see text for details).



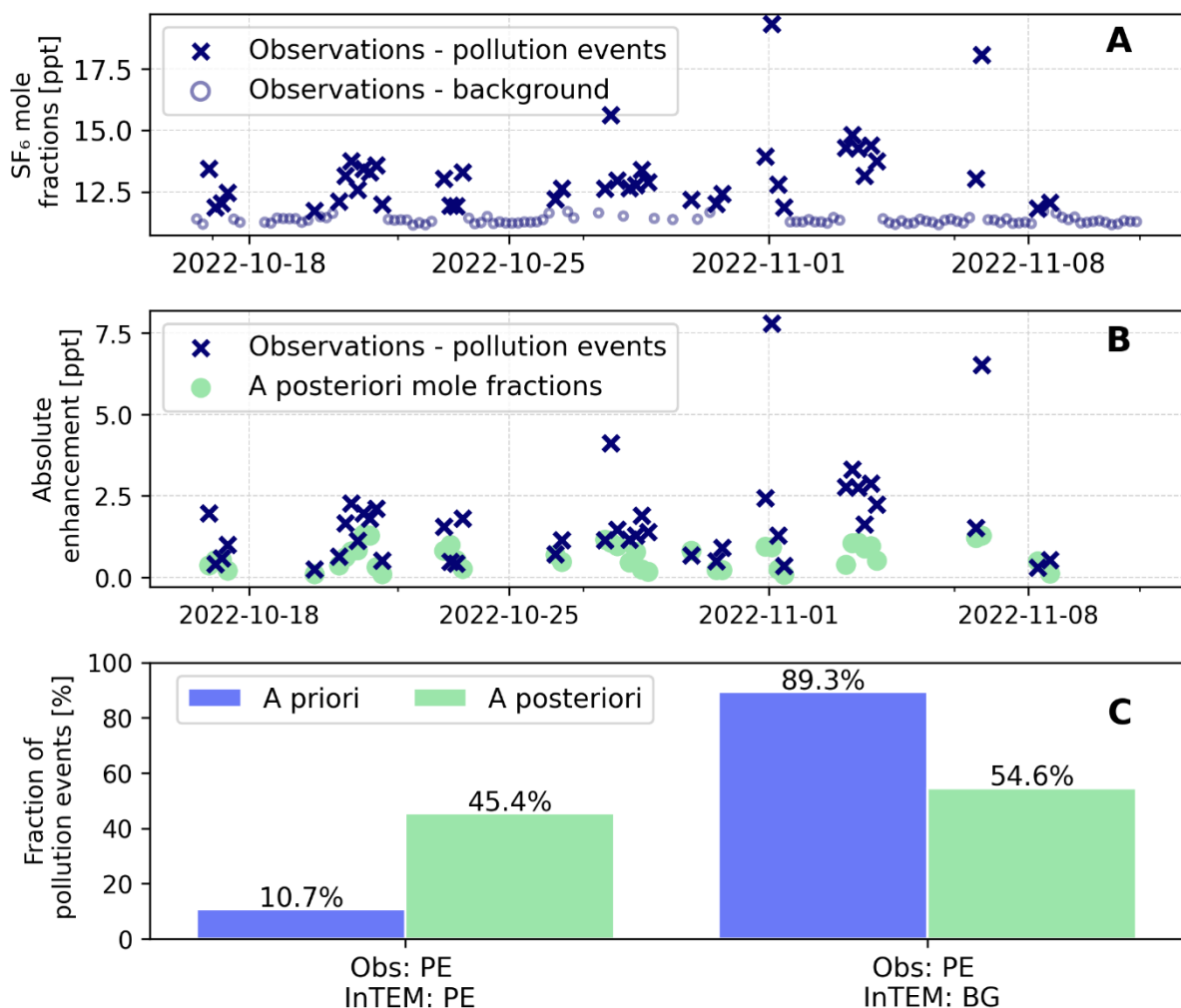
Source: [Meixner et al., 2025]

Figure 6 shows a comparison of a typical period in fall of 2022 from the Taunus Observatory. Panel A shows the observations themselves, Panel B the enhancements above the background in the posterior model data compared to the observed pollution events and Panel C shows some statistics on pollution events captured by the model using the prior emissions field and the posterior emission field in comparison to the observations. Using the prior emissions, only 10.7% of the observed pollution events are also classified as pollution by the model. This fraction increases to 45.4% when using the posterior emission field. By contrast, 89.3% of the observed pollution events could not be reproduced by the model using the prior emissions, while only 54.6% of the observed pollution events are not reproduced by the model using the posterior emissions. Overall, the probability of the model to reproduce an observed pollution event has increased by a factor of more than 4. When comparing the complete datasets, the

correlation coefficient between model and observations improves from 0.48 (prior mole fractions) to 0.63 (posterior mole fractions, meaning that the model is now able to explain 63% of the observed variability while this was only 48% previously. While InTEM does not fully reproduce the magnitude of mole fraction peaks, it thus reliably detects the high pollution events and thus provides a realistic representation of regional emission patterns.

Figure 6: Comparison of observations and model

A: Representative excerpt from the SF₆ measurement time series at TOB between 2022-10-15 and 2022-11-15. B: Comparison of absolute enhancements for statistical identified pollution events within the excerpt shown in A. Observations (dark blue) and posterior mole fractions (light green) are displayed. C: Comparison of the classification of the pollution events (PE) observed at Taunus Observatory as Pollution Event or background (BG) by the model for both a priori, and a posteriori emission estimates.



Source: [Meixner et al., 2025]

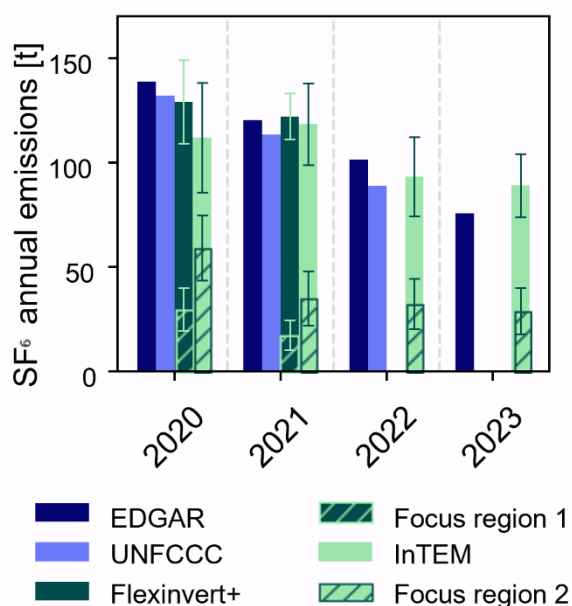
Based on our inversions, the emissions from the point source mentioned have been estimated to be 59 ± 16 tons per year in the year 2020 and about between 29 ± 11 and 35 ± 13 tons per year in the years 2021-2023. The results are compared to the independent inverse modelling study using FLEXPART/Flexinvert+ by (Vojta et al., 2025) mentioned above. Note that for the FLEXPART/Flexinvert+ inversions, the ICOS flask sample data were not used but instead

observations from the station at Ochsenkopf and Schauinsland, so the distribution and density of observations in Germany was more sparse. This study also identifies the emission hot-spot in southwestern Germany, but the attributed emissions are 30 ± 10 tons per year for 2020 and 17 ± 7 tons per year for 2021, thus about 50% smaller than the results from InTEM using our calculations presented here. While the overall emissions from this region derived by FLEXPART/Flexinvert+ are smaller, they mostly agree within the 1 sigma standard deviation and always within the 2 sigma standard deviations. In all cases, the emission hot spot is also clearly identified. All values are compared with bottom-up estimates in table 1.

While we identify an obvious emission hot spot, the total emissions for Germany derived from the inversion are in the same range as those reported to the UNFCCC, in which the mentioned point source is not included (Figure 8). According to the bottom-up emission estimate, which forms the basis of the reporting to the UNFCCC emissions from the decommissioning of soundproof windows are expected to be the main source of SF₆ in Germany. We note, that for such a source, a much more homogeneous distribution of emissions over Germany would be expected (e.g. correlated to population density) than is suggested from our observations and calculations. If the point source mentioned before on the order of 30 tons is added to the current bottom-up emission estimates, these would be larger than the total emissions derived from our inversion calculations. This again would suggest that the main source of SF₆ according to the bottom-up estimation may be overestimated and less SF₆ is emitted from the decommissioning of sound-proof window. This again would indicate that even more SF₆ is still stored in soundproof windows in Germany and the remaining bank might be larger than expected. However, it should be emphasized that there are large uncertainties in both bottom-up and top-down emission estimates, so that this conclusion must be regarded with care and more information on the amount of SF₆- insulated sound proof windows still in use would be needed to sustain this conclusion.

Figure 7: German SF₆ emission estimates (top-down)

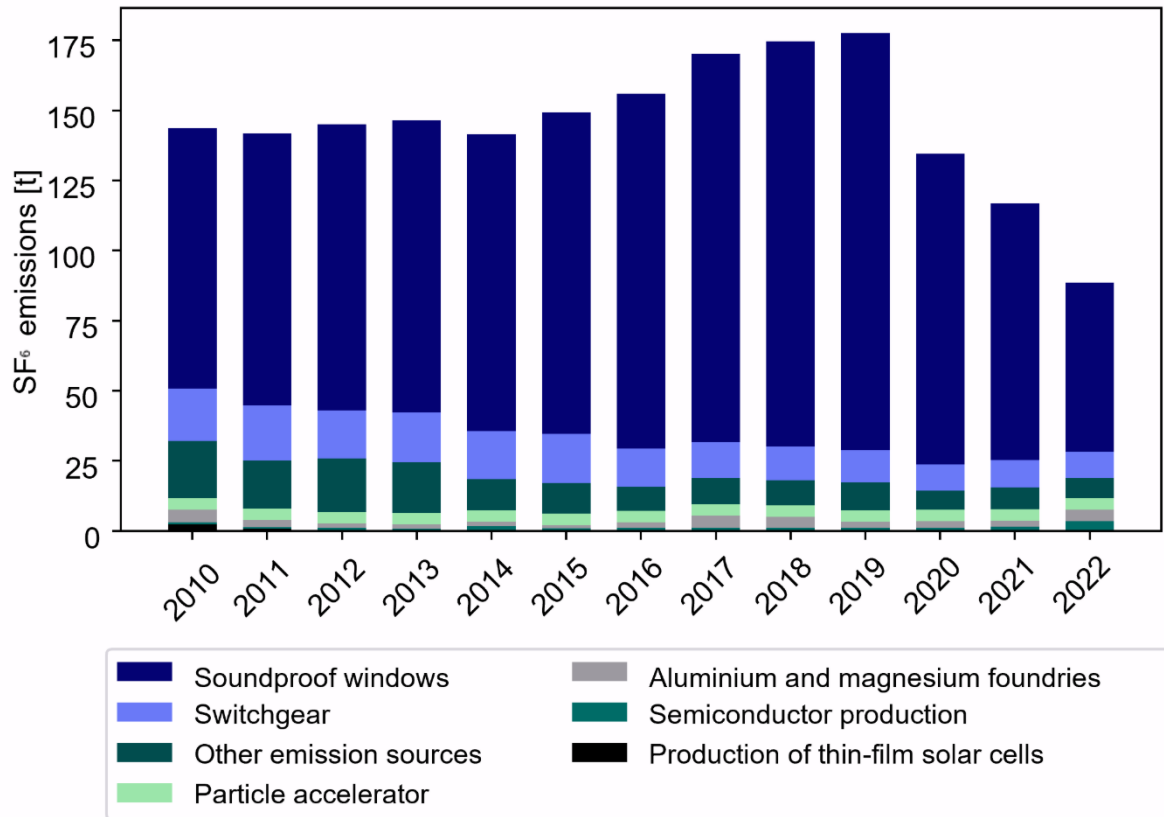
German SF₆ emission estimates [tons per year] from EDGAR (2020 - 2023), UNFCCC inventory (2020 - 2022), Flexinvert+ (2020 - 2021) with focus region 1 (48.75°N - 50.0°N, 8.25°E - 10.00°E) and InTEM (2020 - 2023) with focus region 2 (48.637°N - 49.807°N, 8.404°E - 10.164°E). The error bars describe the 2 σ uncertainty of the ensemble distribution for Flexinvert+ and the InTEM inversion results.



Source: [Meixner et al., 2025]

Figure 8: Reported German SF₆ emissions

Reported bottom-up emissions of SF₆ from Germany to UNFCCC divided by emission category (UBA)



Source: [Meixner et al., 2025]

Table 1: Comparison of top-down (InTEM and Flexinvert) derived emissions of SF₆ with bottom up emission from EDGAR and emissions reported to UNFCC.Comparison of different emission estimates for SF₆; see text for details.

Model	emissions[t]	2020	2021	2022	2023
InTEM (22 european stations)	Germany	112 ± 26	118 ± 20	93 ± 19	89 ± 15
	Focus region	59 ± 16	35 ± 13	32 ± 12	29 ± 11
InTEM (20 european station – excluding TOB and KIT)	Germany	95 ± 25	118 ± 20	94 ± 20	96 ± 16
	Focus region	36 ± 20	37 ± 19	38 ± 19	25 ± 15
InTEM (20 european station – excluding German stations)	Germany	88 ± 30	96 ± 28	77 ± 27	102 ± 21
	Focus region	32 ± 24	47 ± 20	41 ± 18	2 ± 17
EDGAR_2025_GHG	Germany	139	120	101	76
	Focus region	11	9	8	6
Flexinvert+ (Vojta et al 2025)	Germany	119 ± 20	97 ± 10	-	-
	Focus region	28 ± 9	17 ± 5	-	-
UNFCCC	Germany	132	113	88	-

Source: [this project, UNFCC, Vojta et al., 2025]

3.3 Uncertainty of emission estimates

Estimating the model and observation uncertainty is an important part of InTEM and at the same time a challenging task. Uncertainties can arise both from the measurements as well as from the modelling. Observational uncertainty is typically quantified from repeated measurements of the standard gas which is run between ambient air measurements. In the case of the Taunus Observatory Medusa instrument the typical time sequence is to measure a working standard gas and then measure two ambient air samples before the next working standard gas is measured. This working standard (called the quaternary) is measured regularly against a calibration gas tank provided by the central calibration laboratory of AGAGE, which is the SCRIPPS Institute of Oceanography (SIO) at the University of California in San Diego. This calibration gas tank is called as the tertiary and is measured at SIO before shipping to the station and after return from the station. There are two levels of standard (called primary and secondary) at SIO in order to maintain the scale. In the case of SF₆ the scale used is SIO-05. The typical measurement cycle of two standard and two air samples takes about 4 hours; the time difference between standards is thus about three hours. The deviation from the expected value is calculated by deriving the value for each standard measurements from the bracketing standards and then interpolating this onto the air samples. For SF₆ typical reproducibility of this is quoted as 0.6% (Prinn et al., 2018), however, the measurements at Taunus Observatory usually achieve a much better precision, which is about 0.3%, i.e. repeated measurements of the standard only scatter by 0.3% around the mean.

For the model, the standard deviation of the measurements is defined as the observation uncertainty for that day's observations of SF₆ at the station. The second source of uncertainty is

from the model itself. This is defined as having two components: a baseline uncertainty and a meteorological uncertainty. Note that for species like SF₆ chemistry does not play any role, as they are inert over the time periods covered by the inverse modelling calculations. The baseline uncertainty is estimated during the fitting of the northern hemispheric baseline trend to the baseline observations. The meteorological uncertainty stems from uncertainty in the meteorological transport model. This uncertainty is proportional to the magnitude of the pollution event and is set to a minimum of 10% of the size of the enhancement above background. For small enhancements the median pollution event for that gas from the respective year is imposed as a minimum uncertainty.

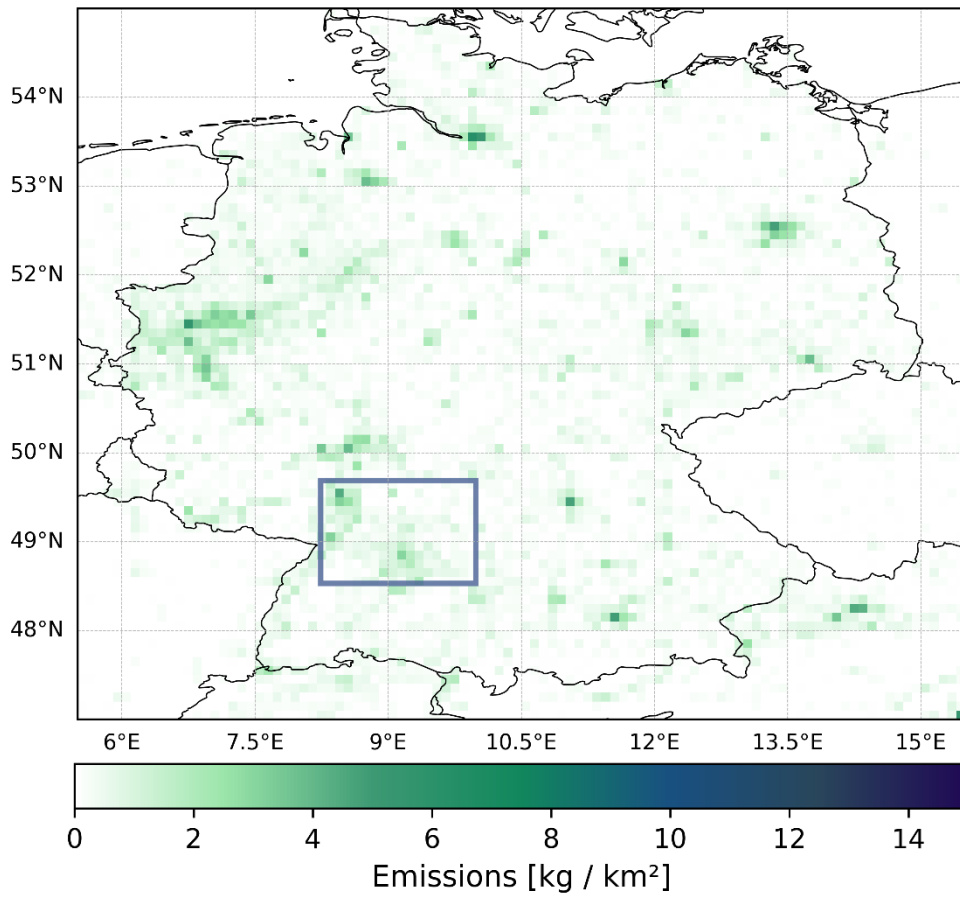
As a further step to ensure a high level of confidence in the inversion results, several criteria are applied to filter the data prior to their use in the inversion. These are essentially four different criteria:

- ▶ The model atmospheric boundary layer is larger than 200 m
- ▶ The model wind speed is above 1.5 m/s
- ▶ The enhancement is not observed in only one grid cell (this is ensured by looking at the deviations to neighbouring grid cells)
- ▶ The vertical temperature gradient is below 1.5 K/km, ensuring that the atmosphere is either near-neutral or unstably stratified.

Using these criteria eliminates data from the inversion which are likely strongly influenced by very local processes, thereby shifting the focus to regional emission patterns.

Next to these uncertainties based on the model and on measurement uncertainties, the prior emission estimates and the distribution of atmospheric observations are key in determining the quality of the estimated emissions. Figure 9 shows the prior distribution of emissions based on the EDGAR emission inventories and distributed within Germany according to population densities. It is clear that this prior distribution differs very significantly from the posterior emission field shown in Figure 5. As a further test of sensitivity we have performed two additional inversions, in which we left out all German observations, respectively only the measurements at Karlsruhe and at the Taunus Observatory (Figure 10). It is clear that the less observations are used, and in particular when leaving out the stations at Karlsruhe and the measurements from the Taunus observatory, the emission hot spot in South-West Germany can be less clearly constrained.

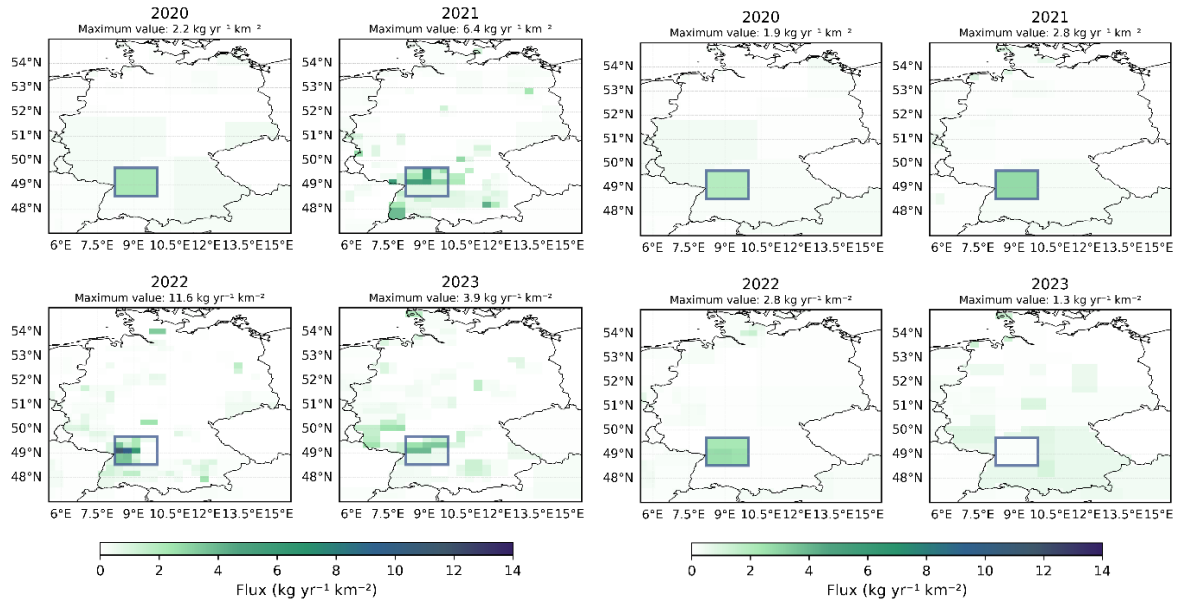
Figure 9: Prior distribution distribution of German annual average SF₆ Emissions based on EDGAR emissions distributed according to population density



Source: [Meixner et al., 2025]

Figure 10: Distribution of German SF₆ Emissions derived from InTEM for the years 2020-2023 with reduced data base

Annual mean InTEM derived emissions for Germany for the years 2020 to 2023 using a reduced data set. Left: same as in Figure 5 but without observations from Taurus and Karlsruhe. Right: leaving out all German emissions. Note that the model cannot allocate the emissions as clearly without these observations.



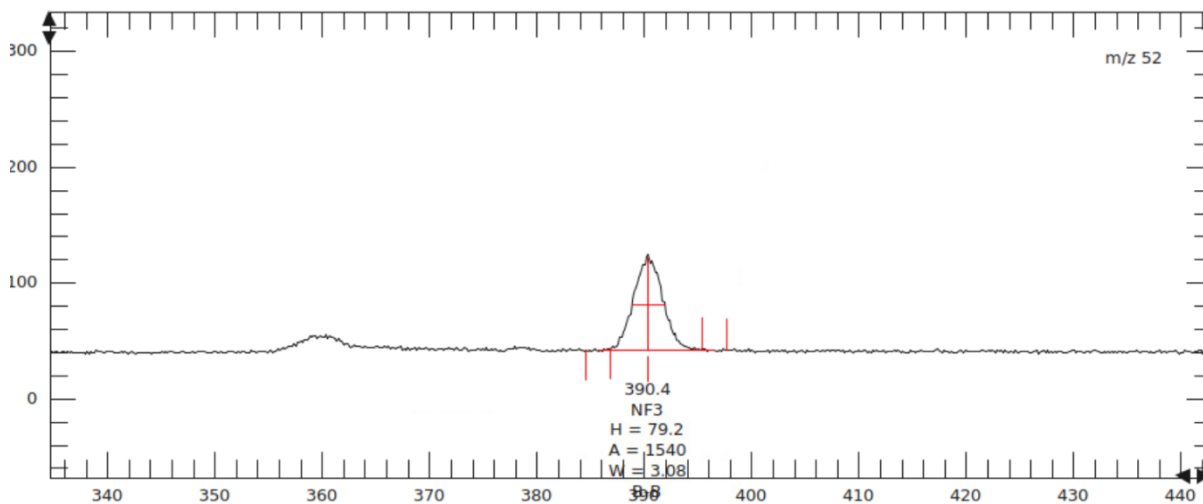
Source: [Meixner et al., 2025]

4 First observations of NF₃ over Germany

As mentioned above, NF₃ is a very potent greenhouse gas and at the same time very difficult to measure. This difficulty in measuring NF₃ arises from its physicochemical behaviour. First, it has a very low boiling point of -129°C and second it has a much lower concentration in the atmosphere than other gases with low boiling points like e.g. Argon and Krypton. Further, there are interferences with CO₂ and it was found that NF₃ can be lost on chromatographic columns (Weiss et al., 2008). Arnold et al. (2013) solved this problem by redesign of the MEDUSA measurement system (Miller et al., 2008), based on the use of a GasPro column. The MEDUSA system installed at the Taunus Observatory on Kleiner Feldberg near Frankfurt is equipped with this redesign and therefore capable of measuring NF₃. All analytical details are in line with the description in (Arnold et al., 2013). As the measurements at the Taunus Observatory are part of the AGAGE network (Prinn et al., 2018), calibration gases for NF₃ are also provided regularly by the Cripps Institute of Oceanography (SIO) of the University of California in San Diego, California. A typical chromatogram of the NF₃ peak is shown in Figure 11.

Figure 11: First Chromatogram of NF₃ from the new Medusa system at Taunus Observatory.

Chromatogram of the first ambient air NF₃ measurements taken on 5th of February 2023 using the newly installed MEDUSA system at Taunus Observatory. NF₃ is detected using the NF₂⁺ fragment at mass to charge ratio of 52. The peak shown here corresponds to a mole fraction of 3.3 ppt in dry ambient air.



Source: [GCWerks software, Goethe University Frankfurt]

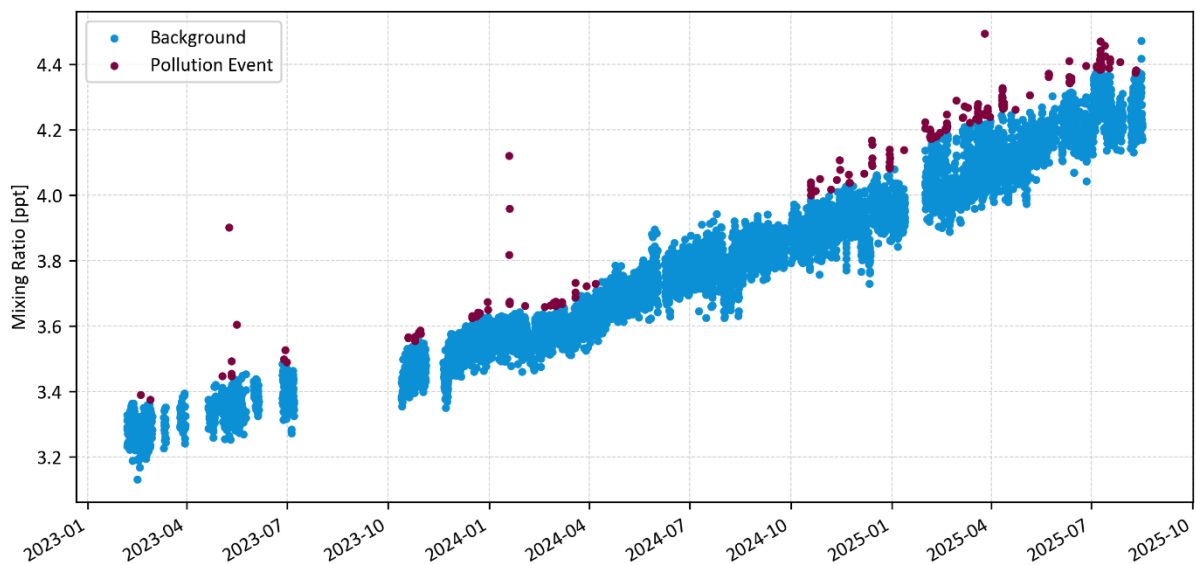
The MEDUSA system at Taunus Observatory was installed in February 2023 and after a range of optimisation measurements first ambient air measurements started in on 5 February 2023. Since then ambient air mole fractions of NF₃ have increased from about 3.3 ppt in February 2023 to about 4.0 ppt in February 2025. Typical precisions for the measurements (1 sigma standard deviations) as derived from the reproducibility of the standard measurements is typically about 1.5%. Some shorter periods were observed with slightly poorer precision of up to 2.5%, sometimes associated with larger fluctuation in the laboratory temperature. Note that this increase is not necessarily related to local or regional emissions, as NF₃ has an atmospheric lifetime in excess of 500 years and background mole fractions and their increase are thus globally very similar. The NF₃ data from the Taunus Observatory (Figure 12) is reported on SIO-

12 scale used by AGAGE (Arnold et al., 2013). Data from the Taunus observatory are included in the regular data reviews which are part of the AGAGE network (Prinn et al., 2018).

Regional and local emissions are reflected in short-term enhancement above this background. Short-term enhancements were observed on three occasions. Two sample in early May 2023 (May, 5th) showed an enhancement of about 0.3, respectively 0.5 ppt above background. Similar short-term enhancements were observed in the night of January 18 to January 19 2024 (three samples) and in March 2025 (one sample with enhancement of about 0.4 ppt). There is no obvious pattern regarding the air mass origin for these three events. It should also noted that compared to many other gases, especially when compared to SF₆ these are very few pollution events and the local enhancements are moderate (for SF₆ occasional enhancements of more than 10 ppt are observed). It is therefore obvious that the sources of NF₃ in the region to which our measurements are sensitive are quite small. Due to the small number of pollution events a quantification of the emissions was not considered reliable.

Figure 12: time series of NF₃ from the new Medusa system at Taunus Observatory.

Measurements of NF₃ at Taunus Observatory (Goethe University Frankfurt). The division into background and pollution was carried out using a data filter developed at the University of Frankfurt (Schuck et al., 2023). Note that only very few measurements are significantly above the background, with two main events (May 2023 and January 2024) and a minor event in March 2025 (this latter event is only one enhanced measurement). Other enhancements above background are not considered to be significant.



Source: [own illustration, Goethe University Frankfurt]

5 List of references

- An, M. D., Prinn, R. G., Western, L. M., Zhao, X. C., Yao, B., Hu, J. X., Ganesan, A. L., Muehle, J., Weiss, R. F., Krummel, P. B., O'Doherty, S., Young, D., and Rigby, M.: Sustained growth of sulfur hexafluoride emissions in China inferred from atmospheric observations, *Nature Communications*, 15, 10.1038/s41467-024-46084-3, 2024.
- Arnold, T., Mühle, J., Salameh, P. K., Harth, C. M., Ivy, D. J., and Weiss, R. F.: Automated measurement of nitrogen trifluoride in ambient air, *Anal. Chem.*, 84, 4798-4804, 10.1021/acs300373e, 2012.
- Arnold, T., Manning, A. J., Kim, J., Li, S., Webster, H., Thomson, D., Mühle, J., Weiss, R. F., Park, S., and O'Doherty, S.: Inverse modelling of CF4 and NF3 emissions in East Asia, *Atmos. Chem. Phys.*, 18, 13305-13320, 10.5194/acp-18-13305-2018, 2018.
- Arnold, T., Harth, C. M., Mühle, J., Manning, A. J., Salameh, P. K., Kim, J., Ivy, D. J., Steele, L. P., Petrenko, V. V., Severinghaus, J. P., Baggenstos, D., and Weiss, R. F.: Nitrogen trifluoride global emissions estimated from updated atmospheric measurements, *Proc. Natl. Acad. Sci.*, 110, 2029-2034, 10.1073/pnas.1212346110, 2013.
- Engel, A., Arduini, J., Arnold, T., Chung, E., Frumau, A., Ganesan, A., Garrard, N., Grant, A., Hermansen, O., Kikaj, D., Lunder, C., Maione, M., Meixner, K., O'Doherty, S., Pitt, J., Reimann, S., Rennick, C., Rigby, M., Safi, E., Say, D., Spain, G., Stanley, K., Stavert, A., van der Bulk, P., Vollmer, M., Wagenhauser, T., Wenger, A., Wisher, A., and Young, D.: Atmospheric measurements results archive from the European AGAGE network, the UK DECC network and the Cabauw tall tower [dataset], 10.18160/ZKVV6-8ZR6, 2024.
- Hu, L., Ottinger, D., Bogle, S., Montzka, S. A., DeCola, P. L., Dlugokencky, E., Andrews, A., Thoning, K., Sweeney, C., Dutton, G., Aepli, L., and Crowell, A.: Declining, seasonal-varying emissions of sulfur hexafluoride from the United States, *Atmospheric Chemistry and Physics*, 23, 1437-1448, 10.5194/acp-23-1437-2023, 2023.
- Kovács, T., Feng, W., Totterdill, A., Plane, J. M. C., Dhomse, S., Gómez-Martín, J. C., Stiller, G. P., Haenel, F. J., Smith, C., Forster, P. M., García, R. R., Marsh, D. R., and Chipperfield, M. P.: Determination of the atmospheric lifetime and global warming potential of sulfur hexafluoride using a three-dimensional model, *Atmos. Chem. Phys.*, 17, 883-898, 10.5194/acp-17-883-2017, 2017.
- Levin, I., Naegler, T., Heinz, R., Osusko, D., Cuevas, E., Engel, A., Ilmberger, J., Langenfelds, R. L., Neininger, B., Rohden, C. v., Steele, L. P., Weller, R., Worthy, D. E., and Zimov, S. A.: The global SF6 source inferred from long-term high precision atmospheric measurements and its comparison with emission inventories, *Atmos. Chem. Phys.*, 10, 2655-2662, 10.5194/acp-10-2655-2010, 2010.
- Manning, A. J., Ryall, D. B., Derwent, R. G., Simmonds, P. G., and O'Doherty, S.: Estimating European emissions of ozone-depleting and greenhouse gases using observations and a modeling back-attribution technique, *J. Geophys. Res.*, 108, 4405, 10.1029/2002JD002312, 2003.
- Manning, A. J., Redington, A. L., Say, D., O'Doherty, S., Young, D., Simmonds, P. G., Vollmer, M. K., Mühle, J., Arduini, J., Spain, G., Wisher, A., Maione, M., Schuck, T. J., Stanley, K., Reimann, S., Engel, A., Krummel, P. B., Fraser, P. J., Harth, C. M., Salameh, P. K., Weiss, R. F., Gluckman, R., Brown, P. N., Watterson, J. D., and Arnold, T.: Evidence of a recent decline in UK emissions of HFCs determined by the InTEM inverse model and atmospheric measurements, *Atmos. Chem. Phys. Discuss.*, 2021, 1-26, 10.5194/acp-2021-261, 2021.
- Meixner, K., Wagenhäuser, T., Schuck, T. J., Alber, S., Manning, A. J., Redington, A. L., Stanley, K. M., O'Doherty, S., Young, D., Pitt, J., Wenger, A., Frumau, A., Stavert, A. R., Rennick, C., Vollmer, M. K., Maione, M., Arduini, J., Lunder, C. R., Couret, C., Jordan, A., Gutiérrez, X. G., Kubistin, D., Müller-Williams, J., Lindauer, M., Vojta, M., Stohl, A., and Engel, A.: Characterization of German SF6 Emissions, *ACS ES&T Air*, 10.1021/acsestair.5c00234, 2025.
- Miller, B. R., Weiss, R. F., Salameh, P. K., Tanhua, T., Grealley, B. R., Mühle, J., and Simmonds, P. G.: Medusa: A sample preconcentration and GC/MS detector system for in situ measurements of atmospheric trace halocarbons, hydrocarbons, and sulfur compounds, *Analytical Chemistry*, 80, 1536-1545, 10.1021/ac702084k, 2008.
- Prinn, R., Weiss, R., Arduini, J., Choi, H., Engel, A., Fraser, P., Ganesan, A., Harth, C., Hermansen, O., Kim, J., Krummel, P., Loh, Z., Lunder, C., Maione, M., Manning, A., Mitrevski, B., Mühle, J., O'Doherty, S., Park, S., Pitt,

J., Reimann, S., Rigby, M., Saito, T., Salameh, P., Schmidt, R., Simmonds, P., Stanley, K., Stavert, A., Steele, P., Vollmer, M., Wagenhäuser, T., Wang, R., Wenger, A., Western, L., Yao, B., Young, D., Zhou, L., and Zhu, L.: Version 20250721 of Dataset published 2025 via NASA Langley Research Center (LaRC) Data Host Facility (DHF) [dataset], 10.60718/75d7-qe84, 2025.

Prinn, R. G., Weiss, R. F., Arduini, J., Arnold, T., DeWitt, H. L., Fraser, P. J., Ganesan, A. L., Gasore, J., Harth, C. M., Hermansen, O., Kim, J., Krummel, P. B., Li, S., Loh, Z. M., Lunder, C. R., Maione, M., Manning, A. J., Miller, B. R., Mitrevski, B., Mühle, J., O'Doherty, S., Park, S., Reimann, S., Rigby, M., Saito, T., Salameh, P. K., Schmidt, R., Simmonds, P. G., Steele, L. P., Vollmer, M. K., Wang, R. H., Yao, B., Yokouchi, Y., Young, D., and Zhou, L.: History of chemically and radiatively important atmospheric gases from the Advanced Global Atmospheric Gases Experiment (AGAGE), *Earth Syst. Sci. Data*, 10, 985-1018, 10.5194/essd-10-985-2018, 2018.

Ravishankara, A. R., Solomon, S., Turnipseed, A. A., and Warren, R. F.: Atmospheric Lifetimes of Long-Lived Halogenated Species, *Science*, 259, 194-199, 1993.

Ray, E. A., Moore, F. L., Elkins, J. W., Rosenlof, K. H., Laube, J. C., Röckmann, T., Marsh, D. R., and Andrews, A. E.: Quantification of the SF₆ lifetime based on mesospheric loss measured in the stratospheric polar vortex, *Journal of Geophysical Research: Atmospheres*, 122, 4626-4638, 10.1002/2016JD026198, 2017.

Rigby, M., Mühle, J., Miller, B. R., Prinn, R. G., Krummel, P. B., Steele, L. P., Fraser, P. J., Salameh, P. K., Harth, C. M., Weiss, R. F., Grealley, B. R., O'Doherty, S., Simmonds, P. G., Vollmer, M. K., Reimann, S., Kim, J., Kim, K. R., Wang, H. J., Olivier, J. G. J., Dlugokencky, E. J., Dutton, G. S., Hall, B. D., and Elkins, J. W.: History of atmospheric SF₆ from 1973 to 2008, *Atmospheric Chemistry and Physics*, 10, 10305-10320, DOI 10.5194/acp-10-10305-2010, 2010.

Schuck, T. J., Degen, J., Hintsä, E., Hoor, P., Jesswein, M., Keber, T., Kunkel, D., Moore, F., Obersteiner, F., Rigby, M., Wagenhäuser, T., Western, L. M., Zahn, A., and Engel, A.: The interhemispheric gradient of SF₆ in the upper troposphere, *EGUosphere*, 2023, 1-25, 10.5194/egusphere-2023-1824, 2023.

Simmonds, P. G., Rigby, M., Manning, A. J., Park, S., Stanley, K. M., McCulloch, A., Henne, S., Graziosi, F., Maione, M., Arduini, J., Reimann, S., Vollmer, M. K., Mühle, J., O'Doherty, S., Young, D., Krummel, P. B., Fraser, P. J., Weiss, R. F., Salameh, P. K., Harth, C. M., Park, M. K., Park, H., Arnold, T., Rennick, C., Steele, L. P., Mitrevski, B., Wang, R. H. J., and Prinn, R. G.: The increasing atmospheric burden of the greenhouse gas sulfur hexafluoride (SF₆), *Atmos. Chem. Phys.*, 20, 7271-7290, 10.5194/acp-20-7271-2020, 2020.

Vojta, M., Plach, A., Thompson, R. L., Purohit, P., Stanley, K., O'Doherty, S., Young, D., Pitt, J., Lan, X., and Stohl, A.: A thousand inversions to determine European SF₆ emissions from 2005 to 2021, *EGUosphere*, 2025, 1-64, 10.5194/egusphere-2025-1095, 2025.

Vojta, M., Plach, A., Annadate, S., Park, S., Lee, G., Purohit, P., Lindl, F., Lan, X., Mühle, J., Thompson, R. L., and Stohl, A.: A global re-analysis of regionally resolved emissions and atmospheric mole fractions of SF₆ for the period 2005-2021, *Atmospheric Chemistry and Physics*, 24, 12465-12493, 10.5194/acp-24-12465-2024, 2024.

Weiss, R. F., Mühle, J., Salameh, P. K., and Harth, C. M.: Nitrogen trifluoride in the global atmosphere, *Geophys. Res. Lett.*, 35, L20821, 10.1029/2008gl035913, 2008.

Weng, W. B., An, M. D., Western, L. M., Prinn, R. G., Hu, J. X., Zhao, X. C., Rigby, M., Wang, Y. N., Huang, S. Y., Xu, H. H., Yu, Y., Chi, W. X., and Yao, B.: Nitrogen Trifluoride Emissions in China from 2017 to 2021 Derived from Atmospheric Observations, *Environ Sci Tech Lett*, 11, 1096-1102, 10.1021/acs.estlett.4c00527, 2024.